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Maryam Heydari, Guillaume Guérin, Mohsen Zeidi, Nicholas Conard. Bayesian luminescence dating at Ghār-e Boof, Iran, provides a new chronology for Middle and Upper Paleolithic in the southern Zagros. Journal of Human Evolution, 2021, 151, pp.102926. 10.1016/j.jhevol.2020.102926. insu-03182238

# HAL Id: insu-03182238 https://insu.hal.science/insu-03182238

Submitted on 3 Feb 2023  $\,$ 

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Bayesian luminescence dating at Ghār-e Boof, Iran provides a new chronology for Middle and Upper Paleolithic in the southern Zagros

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# Acknowledgments

This work is part of Ph.D. thesis of M.H. financed by the Laboratoire d'Excellence Sciences archéologiques de Bordeaux (LaScArBx), a programme supported by the Agence Nationale de la Rerchere (ANR) - n° ANR-10-LABX-52. We are grateful to David Alba, associate editor, and three anonymous reviewers for providing constructive feedback that improved our manuscript. Sebastian Kreutzer is thanked for creating the map and running the IR-RF tests on the system at the Lux laboratory at the Université du Quebec à Montréal (Canada). We are grateful to Michel Lamothe for giving us access to his equipment for the IR-RF tests. Chantal Tribolo is thanked for her constructive comments on an earlier version of the manuscript. Hélène Valladas is thanked for irradiating two samples at the laboratory of Gif-sur-Yvette (Laboratoire des Sciences du Climat et de l'Environnement).

We are grateful to Mohammad Beheshti, the former head of research center at Iran Cultural Heritage, Handicrafts and Tourism Organization (ICHHTO), Hamideh Choubak, the former head of Iranian Center for Archaeological Research (ICAR), Monireh Kholghi, the head of international section at ICHHTO, Alireza Sardari, Ahmad Chaichi, Siamak Sarlak, Mohammad Mortezaei, Hana Bahrani Pour, and Fatemeh Farshi Jalali, at ICAR for facilitating this work and providing the necessary permits. We are also grateful to Mosayeb Amiri, the head of ICHHTO in Fars and Maghamat Mahmoudi, the head of the cultural heritage office of Rostam County for their help and facilitating the work. We thank Rasoul Boroujeni and Kourosh Alamdari, our Iranian representatives, the field crew especially Saman Hamzavi for their work in as members of the excavation team and for their

important contribution to the lab work. The excavation was funded by the Deutsche Forschungsgemeinschaft (DFG) grant CO 226/30-1.

1

#### 2 Abstract

3 Ghār-e Boof is a Paleolithic cave site in Iran well known for its rich early Upper Paleolithic Rostamian 4 assemblages. The site is located on the edge of the Dasht-e Rostam plain in the southern Zagros. 5 Recent excavation by the members of the Tübingen-Iranian Stone Age Research Project (TISARP) at 6 Ghār-e Boof also recovered well-stratified Middle Paleolithic assemblages. Here we provide the first 7 detailed luminescence chronology for the Middle and Upper Paleolithic of the site. More generally, 8 our work is the first luminescence chronology for a Middle and Upper Paleolithic site in the Zagros 9 Mountains region in Iran. The luminescence ages for the Upper Paleolithic of Ghār-e Boof agree with 10 published <sup>14</sup>C dates. We applied Bayesian models specifically designed for luminescence dating using 11 the R package 'BayLum' to incorporate the well-established stratigraphic constraints as well as the 12 published <sup>14</sup>C ages with our optically stimulated luminescence (OSL) ages to improve the precision of 13 the chronological framework. The Bayesian chronology shows a significantly improved precision of the OSL ages in particular for the upper part of the sequence where <sup>14</sup>C ages were available. The 14 15 Bayesian OSL ages for the Rostamian horizons AH III (a-b-c) and AHs IV fall in the range of 37-42 ka 16 (68% CI). Moreover, we determined a series of dates between 45-81 ka (68 % CI) for the Middle 17 Paleolithic strata AH IVd and AH VI. Our results point to a demographic shift in the populations responsible for the Middle Paleolithic and the Rostamian within three millennia. This major 18 19 technological change accompanied by the rise of symbolic artifacts such as personal ornaments, may 20 or may not reflect a replacement of Neanderthals by modern humans. While we are confident that 21 the Rostamian was made by modern humans, available information does not allow us to be sure 22 who made the local Middle Paleolithic.

23

24 Keywords: Luminescence chronology; Bayesian modeling; Paleolithic; Zagros Mountains; Iran.

25

## 26 **1. Introduction**

#### 27 1.1. Aims of this study

28 Chronological studies are an integral part of Paleolithic research to track human evolution over 29 time. Numerous Middle and Upper Paleolithic sites were dated to establish a chronology for the 30 dispersal of anatomically modern human (AMH) from Africa toward central Asia, in particular in the 31 Levant (e.g., Bar-Yosef and Meignen, 2001; Grün et al., 2005; Trinkaus, 2005; Shea, 2003, 2010; 32 Meignen, 2012; Nishiaki and Akazawa, 2018). However, further toward the east, in the vast region of 33 the Zagros Mountains, we still lack reliable chronologies, which hampers a better understanding of 34 the rich archaeological record of the region (Smith, 1986; Shidrang et al., 2016). While fossils of AMH 35 are known in the Zagros Mountains (e.g., site of Wezmeh: Trinkaus et al., 2008; site of Warwasi: 36 Tsanova, 2013), they have been poorly dated.

The Zagros Mountains have been the focus of Paleolithic studies for decades, not only to unravel the Middle and the Upper Paleolithic cultures of this region but also to decipher occupational discontinuity or transition documented in the region (e.g., Biglari, 2001; Jaubert et al., 2006; Conard and Ghasidian, 2011; Shidrang et al., 2016; Heydari-Guran and Ghasidian, 2017; Bazgir et al., 2017).

41 The few dated stratigraphic sequences in the Zagros Mountains rely on <sup>14</sup>C dating. Shanidar cave, 42 with its rich history of study, provided radiometric ages for the Baradostian culture (Solecki 1963; 43 Hole and Flannery, 1968; Solecki and Solecki, 1993; Becerra-Valdivia et al. 2017). Moreover, in addition to the radiocarbon sequence at Ghār-e-Boof (Conard and Ghasidian 2011; Baines et al., 44 2014; Becerra-Valdivia et al. 2017), <sup>14</sup>C dating was also applied at two sites, the Yafteh Cave (Otte et 45 46 al., 2011) and the Kaldar Cave (Bazgir et al., 2017), located in the Central Zagros, to determine ages 47 for the Upper Paleolithic in Zagros. Nevertheless, despite the few successful applications of <sup>14</sup>C 48 dating, the temporal range is technically limited to the early Upper Paleolithic or very late Middle 49 Paleolithic period (ca. 50 ka; Higham, 2011).

In this study, we present a new chronology for the site of Ghār-e Boof located at the south of the Zagros Mountains, obtained by luminescence dating. The site has yielded both Middle and the Upper Paleolithic assemblages (Conard and Ghasidian 2011; Bretzke and Conard, 2017; Conard and Zeidi, 2019; Zeidi and Conard, 2019). It is situated close to a probable passage of AMH, arriving from Africa through the south of the Iranian plateau, according to various dispersal models (Mellars, 2006; Petraglia et al., 2010; Rosenberg et al., 2011; Boivin et al., 2013; Vahdati Nasab et al., 2013).

56 The site of Ghār-e Boof has been excavated and studied since 2006 in the framework of the 57 Tübingen Iranian Stone Age Research Project (TISARP). The rich and distinctive lamellar early Upper 58 Paleolithic assemblage found during the excavation at Ghār-e Boof and during surveys at 88 sites in 59 the Dasht-e Rostam alone stands in remarkable contrast to the Baradostian and the so-called Zagros 60 Aurignacian. This led Conard and Ghasidian (2011) to define a new industry named the Rostamian, 61 after the Dasht-e Rostam Plains (Conard et al., 2013). The Upper Paleolithic sequence of the site was already dated with <sup>14</sup>C dating in several earlier studies (Conard and Ghasidian, 2011; Baines et al., 62 63 2014; Becerra-Valdivia et al., 2017). These results were refined using Bayesian modeling, leading to 64 the earliest Upper Paleolithic settlement between 41,950–39,850 cal BP (68% credible interval [CI]; 65 Becerra-Valdivia et al., 2017). Ghasidian's doctoral research resulted in detailed presentations of the 66 cultural sequence of the Rostamian from Ghār-e Boof (Ghasidian, 2014; Ghasidian et al., 2017) based 67 on the first two seasons of excavation in 2006 and 2007. Fieldwork by the TISARP team in 2015 and 68 2017 extended the stratigraphic sequence to bedrock and uncovered multiple Middle Paleolithic find 69 horizons (Bretzke and Conard, 2017; Conard and Zeidi, 2019; Zeidi and Conard, 2019).

Below, we provide details of the luminescence dating for the Middle and Upper Paleolithic sequence of the site, and we compare the obtained luminescence ages of the Upper Paleolithic with those available <sup>14</sup>C ages. We present the first luminescence-based chronology for the Middle Paleolithic period in the south of the Zagros Mountains. Moreover, our study goes beyond a simple Middle and Upper Paleolithic luminescence chronology for the Zagros Mountains: we also deployed Bayesian modeling as implemented in the R (R Core Team, 2019) package 'BayLum' (Combès et al., 2015, Combès and Philippe, 2017; Philippe et al., 2018) to incorporate all available chronological data (optically stimulated luminescence [OSL] and <sup>14</sup>C ages) for the site of Ghār-e Boof, to render a
 precise chronology covering both the Middle and the Upper Paleolithic periods. The advantages of
 such incorporation in Bayesian School will be discussed.

80

#### 81 1.2. Environmental setting

82 The Dasht-e Rostam region is located in the south of the Zagros Mountains in the northwest of the Fars Province. The province stretches mainly across the Zagros Folded belt. Most of the 83 84 elevations of this belt are comprised of parallel limestone anticlines, which are generally oriented 85 from northwest to southeast (Brookes, 1989; Stöklin and Navabi, 1973). The topography of this area 86 is diverse with various geomorphological features such as mountains ranging from 700 to 2500 m 87 a.s.l., valleys, rivers, and plains (Heydari-Guran, 2014). The area is known to be semiarid to arid, but 88 the presence of the permanent Fahliyan River (Fig. 1) alongside more than 50 springs and seasonal 89 rivers, like Shiv and Solak form a local wetland (Heydari-Guran, 2014). The climate of this region 90 belongs to the mild temperature zone (Bobek, 1968; Ganji, 1968).

91 The geological context in this area comprises the Miocene to the Quaternary, and the Jurassic to
92 the Oligocene (Heydari-Guran, 2014). The rocks of this region are mainly composed of limestone,
93 dolomite and argillaceous limestone, which is a normal pattern for the Zagros Mountains (Ghasidian,
94 2014; Motiei, 1993).

95 Members of the Tübingen-Iranian Stone Age Research Project (TISARP) conducted survey in the 96 Dasht-e Rostam and identified numerous Paleolithic sites in the form of open-air sites, rock shelters, 97 and caves. Study of these lithic artifacts assemblages showed that they mainly originate from the 98 Upper Paleolithic (Conard and Ghasidian, 2011; Heydari-Guran, 2014). According to the distribution 99 of the discovered lithic artifacts from the surface, the region was classified into divided small zones 100 (microhabitats; Heydari-Guran, 2014). One of those zones, which exhibits the highest concentration 101 of lithic artifacts, is the Yagheh Sangar corridor. The pass is situated in the middle of the Dasht-e 102 Rostam, and it connects plains of Dasht-e Rostam I and Dasht-e Rostam II (Fig. 1). This corridor

encompasses several caves, rock shelters, and open-air sites, which contains ca. 33 % of the known Paleolithic sites in the Dasht-e Rostam plains (Heydari-Guran, 2014). The cave of Ghār-e Boof, which is located at an altitude of 905 m a.s.l., 40 m above the valley bottom, is one of these Paleolithic sites, in the center of the Yagheh Sangar corridor.

107 The area inside of the cave is ca. 60  $m^2$ , with a ceiling height of ca. 8 m (Fig. 1). The Fahlian River 108 is located 5 km at the south of the cave, and the seasonal Solak stream is situated within 200 m at 109 the northeast of the cave. Several large boulders at the entrance of the cave protect the deposited 110 sediments inside the cave from being washed away by erosional processes (Conard and Ghasidian, 111 2011, Ghasidian, 2014). These preserved sediments distinguish the site of Ghār-e Boof from the other Paleolithic sites in the region, providing a unique potential for further systematic 112 113 investigations. Surface studies yielded 436 lithic artifacts, categorized by the presence of flakes, 114 blade and, especially, bladelets and bladelet cores (Conard and Ghasidian, 2011; Ghasidian, 2014). 115 The chert from the river of Fahlian was the main source of raw material for producing lithic artifacts. 116 In the following, the observed layers are identified based on geological horizons (GH) and

archaeological horizons (AH). Besides, both GH and AH refer to identical layers but were investigatedusing different approaches.

<u>Stratigraphy</u> The overall sequence at Ghār-e Boof is comprised of nearly 6 m of well-stratified deposits. The geological horizons 1 and 2 (GH1, GH2) at the top of the profile are associated with the Holocene. GH 2 encompasses two sublayers (GH 2a and GH 2b). The bottom of GH 2 (GH 2b) contains limestone cobbles with sizes from 5 to 25 cm in the north and the center of the profile (western wall; Fig. 2). These cobbles separate the Holocene layers from the Pleistocene layers, which start from GH 3 onwards (Ghadisian, 2014).

GH 3, with thicknesses ranging from 10 to 65 cm in different parts of the cave, often contains ashy silt sediments with colors from yellow-brown to light gray. Fragments of limestone are present in this layer. Sublayers GH 3a and GH 3b underlay GH 3 with a thickness of ca. 15 cm and ca. 60 cm, comprised of medium brown ashy silt and dark brown silt, respectively. Both sublayers contain 129 abundant lithic artifacts, faunal remains and pieces of charcoal. Continuing downward, GH 4 consists 130 of yellow-gray silt with a thickness of ca. 15 cm. The density of limestone fragments in this layer is 131 higher than in GH 3. GH 4a with a thickness of ca. 30 cm, is characterized by a mixture of light 132 yellow-brown silt and limestone fragments smaller than 5 cm. GH 4b, that is darker in color than GH 133 4a, and contains light brown silt and pieces of limestone in lower concentration than GH 4a. Finally, 134 GH 5 and GH 6, which correspond to about 2.5 m of deposits overlying the bedrock (Fig. 2), are 135 comprised of light brown to gray silty sediments with a large amount of limestone clasts (Conard and 136 Zeidi 2019; Zeidi and Conard 2019).

137 Archaeological finds The archaeological horizons AH I and AH II contain ceramic and pottery sherds, 138 which are attributed to the historical period (Conard and Ghasidian, 2011). AH III yielded the richest 139 archaeological materials, not only because of the high concentration of lithic artifacts but also 140 because of fragmented but well-preserved animal bones. The botanical remains preserve what 141 appears to be an exceptional record of early dietary plant use during the Rostamian (Baines et al. 142 2014). The lithic artifacts from AH III, which are rich in bladelets and tools made on bladelets, make 143 Ghār-e Boof the type locality for the Rostamian (Conard and Ghasidian, 2011, Conard et al., 2013; 144 Ghasdian, 2014). Moreover, many perforated shells of various species from AH II b to AH IV were 145 used as personal ornaments (Conard and Ghasidian, 2011; Ghasidian, 2014; Conard and Zeidi, 2019). 146 The concentrations of lithic artifacts in the Middle Paleolithic strata of AH IVd-VI are low 147 compared to the extremely rich Rostamian deposits. These layers also contain large amounts of 148 charred botanical remains as well as faunal remains that are currently under study. The Middle 149 Paleolithic assemblages excavated in 2015 and 2017 have thus far only been published in 150 preliminary reports (Bretzke and Conard, 2017; Conard and Zeidi, 2019; Zeidi and Conard, 2019).

151

## 152 **2.** Materials and methods

#### 153 2.1. Sampling

Fourteen sediment samples were taken from the south of the western and northern walls (Fig. 2) starting from AH IIIb on top of the sequence to AH VI right above the bedrock. To protect the stability of the profile, we avoided hammering and collected the samples in opaque bags at night using orange light. For the sampling, first, we cleaned each sampling location and removed a sediment layer of ca. 5 cm to avoid sampling weathered sediments subject to recent long-term exposition to light and air. Then, we collected the sediments by digging into the profile.

160

#### 161 2.2. Sample preparation

162 Sample preparations were carried out following commonly accepted luminescence sample preparation procedures (Preusser et al., 2008) under subdued orange light conditions appropriate 163 164 for luminescence dating (sodium vapor lamp, ca. 589 nm). Wet sieving was performed to extract 165 grains between 41 to 60  $\mu$ m. We have selected this grain-size because it represents the dominant fraction of the material available in (relative) abundance, and the fraction could be prepared in a 166 167 reasonable amount of time. The samples were then treated with HCl (10% and 35%) to dissolve 168 carbonates until no more reaction was observed. The samples were then treated with  $H_2O_2$  (30%) for one week to eliminate organic materials. Then, we divided the prepared sediments into two 169 170 groups: Group 1 was treated using HCl (35 %) at 65 °C for 3 h to remove the iron coating. We 171 retained this part of the so-prepared samples (polymineral) for infrared stimulated luminescence 172 (IRSL) measurements. Group 2 was soaked with a mixture of 90% hexafluorosilicic acid (H<sub>2</sub>SiF<sub>6</sub>, 37%) 173 plus 10% nitric acid (HNO<sub>3</sub> 68%; cf. Frayret et al., 2006 for the procedure) for one week to obtain purified quartz grains. This procedure was followed by another wash in HCl (15%) overnight to 174 175 remove remaining calcium fluorides. Finally, wet sieving was applied again to discard any remaining 176 grains from the mineral group of feldspar as well as removing any aggregated quartz with the size of 177 less than 41 μm. The amount of quartz grains for sample GB12 was negligible. Therefore, we could
178 not perform any measurements on quartz for this particular sample.

179

#### 180 2.3. Instrumentation and source calibration

181 OSL (Huntley et al., 1985) and IRSL (Hütt et al., 1988) were carried out on two Freiberg Instruments lexsyg SMART TL/OSL systems (Richter et al., 2015). For estimation of the equivalent 182 dose (D<sub>e</sub>) of the quartz grains, we used a system equipped with five blue LEDs (458  $\Delta$  10 nm, 183 184 maximum 70 mW cm<sup>-2</sup>) and five infrared LEDs (850  $\triangle$  3 nm, max. 300 mW cm<sup>-2</sup>). The stimulation power was set to 40 mW cm<sup>-2</sup> for blue and 100 mW cm<sup>-2</sup> for infrared during continuous wave (CW) 185 186 stimulation. For estimating the D<sub>e</sub> of the polymineral grain, we employed another system, equipped with ten green LEDs (525  $\Delta$  20 nm, maximum 70 mW cm<sup>-2</sup>) and five infrared LEDs (850  $\Delta$  3 nm, 187 maximum 300 mW cm<sup>-2</sup>) set to 100 mW cm<sup>-2</sup> (infrared) during continuous wave (CW) stimulation. 188 189 The heating rate for TL signal measurements for both blue-OSL and IRSL measurements was 5 °C/s. 190 Luminescence was detected through a UV filter set for blue-OSL measurements (Schott BG 3, 3 mm 191 and Delta BP 365/50 EX) and a blue-violet filter combination for IRSL measurements (Schott BG 39, 3 mm and AHF-BL HC 414/46 and Schott NG 11, 1 mm) in front of a Hamamatsu H7360-02 192 193 photomultiplier tube (PMT). The two readers were equipped with a <sup>90</sup>Sr/<sup>90</sup>Y-source, which were 194 specifically calibrated for our samples due to their small grain size (41–60  $\mu$ m). We used grains from 195 sample GB4 for calibration with quartz grains as well as calibration with polymineral fraction. The 196 samples were first bleached following the procedure of dose recovery test (see Section 2.4) and then were irradiated with an external <sup>137</sup>C gamma-source (Valladas, 1978) in the laboratory of Gif-sur-197 198 Yvette (Laboratoire des Sciences du Climat et de l'Environnement). The quartz grains and the 199 polymineral both received a gamma-dose of 53 Gy. We measured the given dose using a single 200 aliquot regenerative (SAR) dose protocol (Murray and Wintle, 2000) with the same set up as for our 201 measurements (see below). The result showed that the two luminescence readers delivered ca. 8.52

Gy min<sup>-1</sup> (reader used for the quartz measurements) and 9.96 Gy min<sup>-1</sup> (polymineral) to grains of 41–
60 μm.

Several hundred grains, either quartz or polymineral, were mounted on the stainless steel cups using silicon oil and a mask of diameter 1 mm (small size). We measured 30 aliquots per sample for the quartz grains and 15–16 for the polymineral fractions.

For additional radiofluorescence (RF) test measurements in Bordeaux, we employed the system used by Frouin et al. (2017). Radiofluorescence spectrometry measurements were carried out on the lexsyg research (Richter et al., 2013) system of the Lux laboratory at the Université du Quebec à Montréal. The system is similar to the system in Bordeaux but equipped with an Andor SR-163 spectrograph on conjunction with an Andor DU420A-OE CCD camera connected via a glass fiber to the measurement position. The system was wavelength calibrated, and efficiency calibration relied on technical data relayed by the manufacturer.

214

#### 215 2.4. Luminescence signal measurements

We measured luminescence signals of the quartz and polymineral fraction to determine the corresponding equivalent doses. These procedures enable us to compare the final obtained ages from different minerals and protocols and increase the confidence in the luminescence chronology for Ghār-e Boof.

Quartz optically stimulated luminescence We applied a SAR protocol to the quartz samples to 220 221 determine the equivalent doses (D<sub>e</sub>). Quartz blue-OSL signal (detected in the UV wavelength) 222 consists of several signal components (Bailey et al., 1997). However, the SAR protocol is 223 preferentially employed for the fast decaying signal component, the so-called fast component, 224 bleachable within a few seconds (Wintle and Murray, 2006). Therefore, the first step of 225 measurement was to verify whether quartz samples of the site of Ghār-e Boof were dominated by 226 the fast decaying component or not. We compared one sample from the site (GB1) with the 227 calibration quartz (Risø, batch 90; Hansen et al., 2015), which is known to be dominated by the fast component, using blue CW-OSL, and the corresponding luminescence signals were measured in the
 UV. Both signals were then transformed into the pseudo-linearly modulated-OSL, following Bos and
 Wallinga (2012)—for results see Section 3.1.

231 The OSL signal was measured at 125 °C for 40 s following a preheat for 10 s. The test-dose was 232 measured following a cut heat. We employed the Analyst software v. 4.53 (Duller, 2015) for 233 determining the equivalent doses (D<sub>e</sub>). Regenerative dose points were set at 22, 44, 88, 176, and 352 234 Gy following a test dose of 22 Gy for regeneration dose 1 to 5 (R1 to R5). We calculated the signal 235 intensity based on the initial 0.2 s of stimulation, and the background was estimated from the last 10 236 s. An exponential plus linear function was used for fitting the dose-response curves. After delivering 237 the largest regenerative dose point in the SAR sequence (R5), the samples were given a zero dose 238 (R6) to measure the potential effect of charge transfer due to the previous irradiation or stimulation 239 (Wintle and Murray, 2006). After recuperation, the first regenerative point cycle was repeated (R7) 240 to check the efficiency of correction for sensitivity changes. To account for the possibility of 241 potential contamination of the quartz grains by feldspars, we applied an IR depletion ratio test 242 (Duller, 2003) administrating the same dose as for the first regenerative dose at the end of each SAR 243 cycle (R8).

To monitor a dependency of the D<sub>e</sub> upon the preheat temperature, the preheat plateau test was carried out for sample GB4. The minimum preheat temperature was set to 200 °C, then increased by 20 °C at each step to reach a final temperature of 300 °C. We kept the distance between the preheat and the cut-heat temperature constant at 40 °C.

Additional dose recovery tests were performed on samples GB4 and GB8. The natural signals were first bleached for 100 s in a solar simulator, and then the procedure was followed by a pause of 3 h before the samples were bleached again for another 100 s to eliminate potential charge transfer from the shallow traps to the main trap (325 °C trap). Samples GB4 and GB8 received doses of 57 Gy and 67 Gy (close to their paleodose) respectively, using beta-source inside the luminescence reader, then the given doses were measured using the SAR protocol. 254 Polymineral fraction and the infrared stimulated luminescence Feldspar has been extensively used in 255 luminescence dating. Stimulation of this mineral with an infrared wavelength produces the IRSL 256 signal (Hütt et al., 1988), usually measured in the blue-violet wavelength range, which has several 257 advantages over the quartz OSL signal measured in the UV. The IRSL signal saturates at higher doses 258 compared to the quartz OSL, which leads to the extension of the dating range limitation. Moreover, 259 IRSL signal of potassium feldspar is brighter and usually resulting in lower statistical uncertainties 260 (e.g., Li and Li, 2011). However, IRSL signal suffers from athermal fading (e.g., Wintle, 1973; Spooner, 261 1992), e.g., an unwanted loss of the signal of interest. To overcome this problem, several concepts 262 have been proposed either to correct for fading (e.g., Huntley and Lamothe, 2001) or to use signals 263 with a lower rate of fading (Thomsen et al., 2008, 2011; Thiel et al., 2011). These investigations 264 showed that an elevated temperature IRSL signal displays low or even negligible fading (Thomsen et 265 al., 2011; Li and Li, 2011). These concepts resulted in a series of measurement protocols measuring 266 the IRSL signal at elevated temperatures, e.g., 290 °C following IRSL at 50 °C, the so-called post-IR 267 IRSL 290 °C (pIRIR<sub>290</sub>) protocol (Buylaert et al., 2012). The pIRIR<sub>290</sub> signal is believed not to require any 268 fading correction for the doses <400 Gy (Li and Li, 2012; Zhang and Li, 2020). Hence, this signal was 269 measured for all of the samples using the protocol proposed by Buylaert et al. (2012). The setting of 270 this protocol is listed in Supplementary Online Material (SOM) Table S1.

First, dose recovery tests were carried out on two samples: one sample from the top of the sequence (GB1) and the other one from the bottom of the sequence (GB14). The samples were first bleached for 72 h under the solar simulator then the residual doses were measured, which were 3 Gy for sample GB1 and 4 Gy for sample GB14. In the following, samples GB1 and GB14 received doses of 65 Gy and 124 Gy using beta-source inside the luminescence reader, then the given dose was measured using the pIRIR<sub>290</sub> protocol. The residual doses were subtracted from the measured dose.

278

279 2.5. Dose rates

Energy available to luminescence dating is stored in natural minerals (e.g., quartz) mainly due to the emission of alpha and beta particles as well as gamma photons from natural radionuclides in the surrounding sediment along with dose contributions from high-energetic cosmic rays (Aitken, 1985). Additionally, radionuclides inside potassium feldspar and quartz grains result in an internal dose rate contribution. However, the internal dose rate of quartz grains is often negligible in comparison with the internal dose rate of potassium feldspar grains (Mejdahl, 1987; Huntley and Baril, 1997).

286 The main sources of external radioactivity are nuclides of the U and Th decay chain, as well as K. 287 For our study, the concentration of these radioelements was determined using high-resolution, low-288 level background gamma-ray spectrometry (Guibert and Schvoerer, 1991). We have assumed that 289 the true beta-dose rate arose from sediment with the grain size less than 2 mm and between 2mm 290 to 1 cm after Martin (2015) and Tribolo et al. (2017). For our samples, however, the amount of 291 grains between 2mm and 1 cm was negligible compared to the fraction less than 2 mm. Thus, the 292 sediment samples were first sieved using a mesh size of 2 mm; then the smaller size fraction was packed and sealed in boxes of 12 cm<sup>3</sup>. Storage time of at least four weeks ensured a radioactive 293 294 equilibrium between <sup>222</sup>Rn and its daughters (Guibert and Schvoerer, 1991). The obtained equivalent 295 concentrations of U, Th and K were converted to dose rates using the factors tabulated by Guérin et 296 al. (2011). The attenuation of alpha and beta particles was corrected after Guérin et al. (2012). We 297 applied alpha-efficiency values (a-values) of  $0.03 \pm 0.01$  after Mauz et al. (2006) to calculate the 298 alpha-dose rate for the quartz grains. For the polymineral fractions, we calculated the average alpha-299 efficiency and its standard deviation ( $0.093 \pm 0.013$ ) from values presented for pIRIRSL<sub>290</sub> in Schmidt 300 et al. (2018).

Based on a granulometric analysis (see SOM Fig. S1 as an example) and derived pore volume data, we approximated that a value of  $15 \pm 6$  % would best represent the past water content. This value was increased to  $20 \pm 8$  % for the last two samples (GB13 and GB14), which were taken from GH 6 because of markedly higher water content observed at this particular layer. The uncertainty on 305 water content was set to 40%; this relatively large value was chosen to cover a wider range of water 306 content values. To correct dose rates for the water content, we applied values tabulated in Aitken 307 (1985), Nathan and Mauz (2008) and Guérin and Mercier (2012) for alpha and beta particles, and 308 gamma photons respectively.

The internal dose rate for the quartz grains was calculated using nuclide concentration values from Vandenberghe et al. (2008). For feldspar grains in the polymineral fractions, we assumed an internal K concentration of  $10 \pm 2\%$  after Smedley et al. (2012), and accordingly, we estimated the internal dose rate (Rb was taken into account with a concentration of  $370 \pm 74$  ppm following Mejdahl, 1987) using the conversion factors of Guérin et al. (2011) and corrected for the self-dose fraction after Guérin et al. (2012).

The in situ gamma dose rate was measured for nine samples (GB1 to GB9) using Al<sub>2</sub>O<sub>3</sub>:C chips following the procedure of Kreutzer et al. (2018). The chips were heated to 350 °C for 10 min before being dispatched. Each aluminum tube contained three chips. The tubes stayed in the sediment 720 days (within 5 cm horizontal distance from the location of the corresponding sample). For samples GB10 to GB14, the gamma-dose rates were derived from radionuclide concentrations of K, U and Th obtained by gamma-ray spectrometry (see Section 2.6).

The cosmic-dose rates were calculated after Prescott and Stephan (1982) and Prescott and 321 Hutton (1994). For the calculation, we used a self-written Microsoft Excel<sup>™</sup> sheet. It was designed to 322 323 estimate the cosmic dose rate from four different directions, two sections from the cave entrance 324 and two other sections form the rear of the cave. For each section, the cosmic dose rate was 325 estimated based on nine subsections (in the spherical coordinate system from 0° to 10°,10° to 20° to 326 finally 80° to 90°). We then summed the dose rate estimated from each 10° representing the dose 327 rate of each section. The final dose rate is the sum of the dose rate from all four sections. For 328 estimating the overall uncertainty, we have employed 10% after Prescott and Hutton, (1994) on the 329 final dose rate estimation. To calculate the total dose rate (D<sub>r</sub>), we used a self-written Microsoft  $\mathsf{Excel}^{\mathsf{TM}} \mathsf{ sheet}.$ 330

331 Radioactive disequilibrium Equilibrium in the U decay chain is an underlying fundamental assumption 332 to estimate the dose rate. However, due to the mobility of some of the radionuclides in a particular 333 environmental setting, radioactive disequilibria can be observed. Typical sources of radioactive disequilibria are: (1) <sup>234</sup>U (preferentially over <sup>238</sup>U) can form water-soluble oxidation compound 334 (Krbetschek et al., 1994) that might be transferred and accumulated in other layers; (2) Ra is soluble 335 and chemically active, and can be leached; (3) entrance of soluble <sup>210</sup>Pb in soil water; and (4) loss of 336 337 <sup>222</sup>Rn (gas) due to large pores. One of the typical ways to monitor the possibility of disequilibria in <sup>238</sup>U decay chain is to estimate the effective <sup>238</sup>U content from the top of the chain (pre-<sup>226</sup>Ra) and 338 from the bottom (post-226Ra), which accounts for the potential high chemical mobility of 226Ra 339 (Guibert et al., 2009). To better illustrate the probable radioactive disequilibrium in the <sup>238</sup>U decay 340 chain, the effective <sup>238</sup>U concentrations from the top and the bottom of the U-series were 341 normalized to <sup>232</sup>Th, which is believed to be chemically immobile, to provide a better indicator of 342 343 radionuclides movement in <sup>238</sup>U following the approach of Guibert et al. (2009). The figure is shown 344 in the results section.

345

#### 346 2.6. Combining quartz ages with the radiocarbon ages in 'BayLum'

347 The R (R Core Team, 2019) package 'BayLum' provides an environment for Bayesian data analysis in luminescence dating (Philippe et al., 2018; Christoph et al., 2019; for an application see Heydari et 348 349 al., 2020). However, 'BayLum' is also capable of combining available chronological information, in particular, stratigraphic constraints and <sup>14</sup>C dates with OSL ages to improve luminescence 350 351 chronologies. This may be considered as the most important advantage of performing data analysis 352 in a Bayesian framework (although gains in precision and accuracy have already been demonstrated 353 when using the models implemented in 'BayLum'; Heydari and Guérin, 2018) since it had the 354 potential to lead to more precise chronologies (e.g., Rhodes et al., 2003; Millard et al., 2006; Guérin et al., 2015). Integrating OSL ages with <sup>14</sup>C dates for one specific site in 'BayLum' can reduce the 355 effect of shared systematic errors between the samples in OSL dating. Systematic errors affecting 356

357 series of OSL ages can be modeled using the concept of the covariance matrix, which is named theta 358 matrix in 'BayLum' (Combès and Philippe, 2017). The uncertainty on the calibration of gamma-ray 359 spectrometry, for measuring beta and gamma dose rate as well as the uncertainty on the beta-360 source of the luminescence reader are the main sources of uncertainty inserted into the theta matrix 361 for our study (for full implementation see Heydari et al., 2020). However, for 11 out of 13 quartz 362 samples we employed in situ gamma dose rate measurements while for the two last samples, we 363 used values derived from gamma-ray spectrometry (see Section 4.2). We did not consider the 364 systematic source of uncertainty for the alpha dose rate due to its low contribution compared to the total external dose rate (see Section 3.2). 365

The input for running the model in 'BayLum' is raw data in the form of BIN/BINX-files and the associated information such as channel integrals, the dose rate of the luminescence reader and the environmental dose rate. We assumed that the Gaussian distribution is a representative model to illustrate the equivalent doses (Guérin et al. 2017; Heydari and Guérin, 2018). The uncalibrated <sup>14</sup>C ages with the corresponding uncertainty published in Conard and Ghasidian (2011), Baines et al. (2014) and Becerra-Valdivia et al. (2017) were also combined with the OSL ages and calibrated using IntCal13 (Reimer et al., 2013). For all calculations, the stratigraphic order constrained the modeling.

**374 3. Results** 

#### 375 3.1. Equivalent dose

376 <u>Quartz equivalent dose</u> The results of transformed signals into the pseudo-linearly modulated-OSL 377 from the calibration quartz and sample GB10 are shown in SOM Figure S2. The perfect match of the 378 two curves indicates that the fast signal component dominates the quartz of the samples of Ghār-e 379 Boof.

In the SAR protocol the normalized recuperation signal to the natural signal was always less than
5% for our samples. The recycling ratio (R7/R1) was less than one, and the average of these ratios for

our samples ranged from  $0.82 \pm 0.00$  (for sample GB7) to  $0.87 \pm 0.02$  (for sample GB6). The averages of these ratios for all samples are listed in SOM Table S2. The average of the IR depletion ratios (R8/R7) for each sample ranged from  $0.977 \pm 0.008$  to  $0.991 \pm 0.003$ . These results indicate that the quartz samples were not contaminated with feldspar.

386 Typical dose-response curves and luminescence signals from quartz are shown in Figure 3a as 387 examples. We have also illustrated the TL curves from blue-OSL to visualize the preheat.

388 The result of the preheat measurements is shown in SOM Figure S3; each point represents the 389 average of De after measuring 5 aliquots. The figure illustrates a plateau from 220 to 260 °C, 390 indicating that these temperatures can be used for preheat. We selected a preheat temperature of 391 260 °C for our measurements. The dose recovery ratio resulted in 1.12  $\pm$  0.04 and 1.12  $\pm$  0.05 392 (average of three measured aliquots). We tried to modify the preheat and the cut-heat 393 temperatures to improve the dose recovery ratio and found that a preheat temperature of 280° C 394 and test dose cut heat of 260°C (henceforth 280–260 °C) led to the best dose recovery ratios of 1.01 395  $\pm$  0.01 and 1.00  $\pm$  0.03 for GB4 and GB8 (average of three measured aliquots). We also performed a 396 preheat plateau test for this protocol on sample GB8. The preheat varied from 220°C to 280°C with the cut heat set to 20 °C less than the preheat at each step. 397

398 The result of this preheat test is shown in SOM Figure S4. This figure illustrates that the measured 399 D<sub>e</sub> using the 280–260 °C protocol appears not to be located in the plateau. Therefore, we continued 400 our measurement using 260–220 °C protocol. However, we determined the equivalent doses using 401 the 280–260 °C protocol for three samples GB1, GB4 and GB8 and divided the obtained  $D_e$  from the 402 260–220 °C protocol to the corresponding  $D_e$  obtained derived from the 280–260 °C protocol. The 403 ratios were 1.00  $\pm$  0.03, 1.00  $\pm$  0.03 and 1.01  $\pm$  0.03 for samples GB1, GB4 and GB8 respectively, i.e., 404 indistinguishable from unity. Therefore, we concluded that for our samples, the dose recovery test is 405 not a good representative to test the suitability of the SAR protocol parameters. This observation is 406 in agreement with Guérin et al. (2015), who showed that dose recovery might not be a strong 407 indicator of the accuracy of the measurement protocol settings.

408 Polymineral equivalent dose We obtained dose recovery ratios of 0.99 ± 0.02 for sample GB1 and 409  $0.97 \pm 0.3$  (average of three measured aliquots) for sample GB14 and thus within 10% of unity. The 410 proportions of the test dose to the given dose were 44% for sample GB1 and 23% for sample GB14. 411 These results agree with the findings by Colarossi et al. (2017), who suggested that the ratio of the 412 test dose to the given dose in the pIRIR<sub>290</sub> signal should not be less than 15%. Besides the average of 413 recycling ratios for our samples here ranged from  $0.99 \pm 0.06$  (for sample GB6) to  $1.05 \pm 0.01$  (for sample GB5). Contrary to quartz samples, recycling ratios for polymineral were within 5% of unity. 414 415 The average of the recycling ratios (for consistency with blue-OSL measurements) for all samples are 416 summarized in SOM Table S3.

417 Typical dose-response curves and luminescence signals from sample GB1 are shown in Figure 3b
418 as examples. We have also illustrated the TL curves from pIRIRSL<sub>290</sub> to visualize the preheat.

419 Scatter in the equivalent dose distributions The distributions of the D<sub>e</sub> for both, quartz and 420 polymineral, are exemplarily displayed for samples GB3 and GB14 as Abanico plots (Dietze et al., 421 2016) in Figure 4a–d. The D<sub>e</sub> distributions for all samples are provided in the SOM Figures S5 and S6. 422 Additionally, we have calculated the overdispersion for each D<sub>e</sub> distribution (SOM Table S4) after 423 Galbraith et al. (1999). The D<sub>e</sub>s are quoted as arithmetic average ± the standard error of the mean. 424 The D<sub>e</sub>s of the quartz grains and polymineral fractions ranged from 55 ± 1 to 104 ± 3 Gy and from 65 425 ± 2 to 124 ± 3 Gy, respectively (Table 3).

To justify the use of the arithmetic average for calculating the central dose, despite observing the scatter within aliquots (Fig. 4; for complete version see SOM Figs. S5 and S6), we have, additionally, calculated the central dose using the average dose model (ADM) after Guérin et al. (2017). In this model, the uncertainty on each  $D_e$  is considered to provide the final central dose. These results are listed in SOM Table S5. This table shows that the arithmetic average and the ADM lead to almost identical results. Thus, the arithmetic average is an appropriate measure for this dataset despite the observed scattering between aliquots.

433

434 *3.2. Dose rate* 

The equivalent concentrations of U, Th and K, as well as the calculated external and total dose rates, are shown in Table 1 and 2, respectively. The internal dose rate for quartz and polymineral grains were estimated using DRAC v. 1.2 (Durcan et al., 2015) resulted in 0.01 ± 0.00 and 0.18 ± 0.04 Gy ka<sup>-1</sup>. The external alpha dose rates varied between 0.04 ± 0.01 and 0.06 ± 0.01 Gy ka<sup>-1</sup> for the quartz grains and between 0.13 ± 0.02 and 0.20 ± 0.03 Gy ka<sup>-1</sup> for the polymineral fractions. The external beta dose rates ranged from 0.53 ± 0.02 to 0.89 ± 0.05 Gy ka<sup>-1</sup>.

The in situ gamma dose rate for samples GB1 to GB9 varied between 0.40  $\pm$  0.03 to 0.49  $\pm$  0.03 Gy ka<sup>-1</sup>, which is in good agreement within uncertainties with the corresponding gamma-dose rates derived by laboratory gamma-ray spectrometry, which ranged from 0.35  $\pm$  0.01 to 0.47  $\pm$  0.02 Gy ka<sup>-1</sup> (for samples GB1 to GB14). The final dose rate for the quartz grains ranged from 1.02  $\pm$  0.03 to 1.55  $\pm$  0.06 Gy ka<sup>-1</sup> and correspondingly for potassium feldspar ranged from 1.29  $\pm$  0.05 to 1.81  $\pm$  0.07 Gy ka<sup>-1</sup>.

447 To address figuratively possible radioactive disequilibria, we have plotted the ratio of effective U concentration derived from the top of the chain (pre-<sup>226</sup>Ra) as well as from the bottom of the chain 448 (post-<sup>226</sup>Ra) divided by <sup>232</sup>Th as it was mentioned in Section 2.5. In Figure 5, most of the samples lie 449 close to the equilibrium line. However, the effective <sup>238</sup>U concentrations estimated from the top of 450 451 the chain are higher (from ca. 1.2 times to a maximum of 1.9 times) than the corresponding contents 452 from the bottom of the chain for samples GB2, GB4, GB7, GB10, GB13, and GB14. Unfortunately, it is not straightforward to distinguish whether the source of disequilibria can be attributed to the top or 453 454 from the bottom of the U chain. Hence, we have decided to calculate the average of the effective <sup>238</sup>U from the top and the bottom of the chain for samples GB2, GB4, GB7, GB10, GB13, and GB14 455 456 and presented the dose rate according to the average. However, if we assumed that the disequilibria 457 happened recently in the top of the chain then considering the lower effective U concentration from the bottom, would lead to older ages, from 1% to a maximum of 7%. Likewise calculating the ages 458 459 from the effective U concentration from the top of U chain compared to the average would lead to

460 younger ages, from 1% to a maximum of 6%. However, these differences do not have a significant461 effect on the overall Paleolithic interpretation.

462

#### 463 3.3. Quartz and polymineral ages

Blue-OSL ages from the quartz samples alongside pIRIR<sub>290</sub> ages from the polymineral samples within their standard errors (68% confidence interval) are shown in Figure 6. The figure also presents the calibrated <sup>14</sup>C ages after Baines et al. (2014) and Becerra-Valdivia et al. (2017)— the calibrated ages are taken from Ghasidian et al. (2019). We split those ages into two groups associated with the year of their publication: <sup>14</sup>C (2014) and <sup>14</sup>C (2017) in the legend of Figure 6. The names of archaeological layers in which the samples were taken are displayed next to each sample's name.

470 At first glance, a perfect agreement between the quartz ages and the polymineral ages is 471 observed for almost the entire sample set. Both quartz and polymineral ages smoothly increase with 472 depth. Moreover, the <sup>14</sup>C ages agree with the luminescence ages from the top of the sequence.

473

#### 474 3.4. Infrared radiofluorescence tests on the polymineral fraction

475 We employed infrared radiofluorescence (IR-RF; Trautmann et al., 1998, 1998) using the protocol 476 suggested by Frouin et al. (2017) on two polymineral samples (GB2 and GB14). Unfortunately, the 477 determined D<sub>e</sub>s significantly overestimate those values obtained with the pIRIR<sub>290</sub> protocol (values 478 not shown). To rule out insufficient luminescence signal bleaching as a potential (but here unlikely) 479 cause for this overestimation, we additionally recorded RF spectra (see SOM Fig. S7 as an example 480 for sample GB2) using again the protocol by Frouin et al. (2017). These measurements revealed that 481 the RF spectra are dominated by a strong red emission, while the here relevant IR emission is not 482 distinguishable from background noise, i.e., the polymineral samples from Ghār-e Boof are 483 unsuitable for IR-RF dating; thus, this approach was not further followed up.

484

#### 485 3.5. Bayesian ages

Figure 7 illustrates the result of quartz ages combined with the <sup>14</sup>C dates using 'BayLum'. We did 486 not have OSL samples from AH III; thus the OSL ages start from sublayers IIIa, IIIb and IIIc, which 487 488 resulted in 37–39 ka (68% CI) following 40–41 ka and 40–42 ka corresponding to the sublayers AH IV 489 and AH IVa. Combining the OSL ages with <sup>14</sup>C dates resulted in 35–42 ka for AH III to AH IV (and 490 sublayer IVa). Afterwards, the Middle Paleolithic ages started from sample GB6 with the age of 45-491 48 ka, continuing to the oldest sample of the sequence GB14 with the age of 75-81 ka. The 492 convergence of the Markov chain Monte Carlo (MCMC) along with the age probability density are 493 plotted for sample GB4 in SOM Figure S8 as an example. The Bayesian process converged after 494 4,000,000 iterations.

495

#### 496 **4. Discussion**

#### 497 4.1. Reliability of luminescence ages

498 The OSL age results derived from the quartz grains are in good agreement with the pIRIR<sub>290</sub> ages 499 from the polymineral fractions. The only exception was observed for sample GB8, for which the 500 average of the confidence interval of the  $pIRIR_{290}$  represents an age ca. 10% older than for quartz. A 501 residual dose (hard bleachable signal) might be a reason for the older age of the polymineral 502 compared to the quartz age. The measured residual doses for two samples of GB1 and GB14 were 503 less than 4 Gy and, hence, not significant in comparison with the equivalent doses of 68 Gy and 124 504 Gy. However, there is no indication that laboratory bleaching is equivalent to the natural bleaching 505 before sediment deposition. The residual doses obtained in our study agree with values published in 506 Buylaert et al. (2012) considering well-bleached samples. The excellent agreement between the 507 quartz ages in comparison with the corresponding polymineral ages suggests that the quartz and 508 potassium feldspar grains in the polymineral were sufficiently bleached (Murray et al., 2012).

The probable critical point regarding the blue-OSL ages might be the poor recycling ratio (up to 13–18% lower than unity). These values are lower than what is usually accepted (within 10% of unity) as a standard criterion (Wintle and Murray, 2006). However, here the good match between blue-OSL ages with pIRIR<sub>290</sub> ages (on top of a good agreement with <sup>14</sup>C results) gives confidence on the accuracy of these ages.

514 To see the dependency of estimated D<sub>e</sub> on the recycling ratio, additionally, we categorized the D<sub>e</sub> 515 distribution of each sample (for six randomly selected samples, GB1, GB3, GB5, GB8, GB10, GB14) 516 based on their recycling ratios into two groups: group 1 with recycling ratios less than its average 517 alongside group 2 with recycling ratios larger than its average. The results listed in SOM Table S6, 518 indicate no difference between the D<sub>e</sub> of group I and 2 is observed for samples GB5 and GB8. The 519 discrepancies between the D<sub>e</sub> of two groups corresponding to GB10 and GB14 are negligible. Yet, the 520 observed D<sub>e</sub> differences from samples GB1 and GB3 are more noticeable compared to the other 521 samples; however, within uncertainties, they agree with one another. More importantly, the Des 522 calculated from both groups for GB1 and GB3 show no correlation between low or high recycling 523 ratio and the smaller or larger D<sub>e</sub>. We, therefore, conclude that for our samples, neither low nor high 524 recycling ratio result in significant D<sub>e</sub> underestimation or overestimation.

525 Besides, it appears that the <sup>14</sup>C ages published in Baines et al. (2014) agree more with the OSL 526 ages in comparison with the two ages published in Becerra-Valdivia et al. (2017). These <sup>14</sup>C ages 527 increase gradually with depth and provide the same pattern as for the OSL ages. For layer III (the 528 first layer in the plot) it appears that the age of Baines et al. (2014; calibrated from Ghasidian et al., 529 2019) is more consistent with the luminescence ages and it is likely that the <sup>14</sup>C age of layer III 530 (Becerra-Valdivia et al., 2017) is slightly older. Besides, the age of IVa (Becerra-Valdivia et al., 2017) 531 appears to be younger in comparison with luminescence ages. Finally, the good match of the two 532 distinctly obtained series of luminescence ages (quartz and polymineral), and the consistency of the 533 OSL ages with the <sup>14</sup>C ages provide reasonable confidence in the chronology for the top of the 534 sequence. For ages in the lower profile, OSL and pIRIR<sub>290</sub> ages agree with each other and are stratigraphically consistent. 535

536

#### 537 4.2. The Bayesian approach toward more precise ages

538 In Section 3.5, we combined the OSL ages with the available <sup>14</sup>C ages (Conard and Ghasidian, 539 2011; Baines et al., 2014; Becerra-Valdivia et al., 2017) to build up the Bayesian chronology using the 540 R package 'BayLum'. The correlation between OSL samples due to shared systematic error from the instruments was addressed by creating a theta matrix. For all OSL dating measurements (both the 541 542 equivalent dose and the dose rate), the same instruments were employed except for the in situ 543 gamma-dose rate. We noticed that the gamma-dose rate of samples GB10 and GB11 ( $0.43 \pm 0.02$ 544 and  $0.39 \pm 0.01$  Gy ka<sup>-1</sup>, respectively) deduced from laboratory measurements agreed with the in situ 545 gamma-dose rate of sample GB9 (0.40  $\pm$  0.03 Gy ka<sup>-1</sup>), which is in close location to samples GB10 and 546 GB11 in the profile with in situ gamma dose rate available (Fig. 2). Therefore, for these two samples, 547 we have employed the in situ gamma-dose rate of sample GB9. We have provided one theta matrix considering (1) the uncertainties of in situ gamma-dose rates for samples GB1 to GB11, and (2) the 548 549 uncertainties of gamma-ray spectrometry for samples GB13 and GB14. We did not employ the in situ 550 gamma-dose rate of sample GB9 for samples GB13 and GB14 at the bottom since the environmental 551 situation is completely different with the rest of samples due to presence of a large rock in AH VI and 552 being close to the bedrock (Fig. 2).

553 Comparing Bayesian chronology in Figure 7 with the classical quartz ages in Figure 6 shows that 554 the Bayesian age intervals were considerably reduced, especially for the top of the sequence where 555 <sup>14</sup>C ages are available. To better illustrate the improvement of the uncertainty in the Bayesian 556 chronology, in Figure 8 we show classical quartz ages from Section 3.3 and the Bayesian quartz ages 557 (Section 3.5). The credible intervals created by the Bayesian approach are considerably smaller than 558 those confidence intervals of the classical approach. These reductions are significant (from 57% to a 559 maximum of 73%) where <sup>14</sup>C ages are combined with the OSL ages (from GB1 to GB4). Our results show that combining OSL ages with <sup>14</sup>C ages in the Bayesian modeling when stratigraphic constraints 560 561 were also included indeed result in more precise chronologies. However, for GB6 to GB14, where no

562 <sup>14</sup>C ages were available, Bayesian modeling provides more precise ages by reducing the uncertainties 563 (from 17% to a maximum of 40%). Heydari et al. (2020) observed similar improvements in the 564 precision of the Bayesian chronology caused by stratigraphic ordering even where only OSL ages are 565 involved. In that study, the authors emphasized the effect of applied stratigraphic constraints 566 leading to a reduction of overall uncertainty where samples' age intervals overlap one another. In 567 our study, the stratigraphic order also plays a role, in particular for sample GB1 to GB4, where their 568 age intervals overlap. However, the other reason for the uncertainty reduction is the inclusion of the 569 <sup>14</sup>C ages as independent ages, since such combination, corrects the effect of systematic errors in OSL 570 dating and resulted in ages that are more precise.

571 Moreover, the result of the Bayesian chronology ended up with ages sometimes younger (like 572 GB2 and GB9) and sometimes older (GB7, GB10 and GB11) than the corresponding ages produced by 573 the classical approach of data analysis to satisfy the stratigraphic constraints. Besides, applying 574 stratigraphic constraints for samples GB13 and GB14, which belong to one layer, results in a younger 575 age for sample GB13 and older age for GB14. On the other hand, the classical ages show that the age 576 of GB14 is slightly younger than GB13. As a result, it can be concluded that applying stratigraphic ordering might lead to underestimated or overestimated ages when age intervals overlap. Here we 577 578 believe that this discrepancy is not critical since the Bayesian ages overlap and they statistically are 579 not distinguishable.

580

#### 581 4.3. The obtained chronology in its Paleolithic context

582 Ghār-e Boof is mainly recognized for its rich Upper Paleolithic assemblages based on bladelet 583 production named Rostamian tradition (Conard and Ghasidian, 2011, Ghasidian, 2014; Ghasidian et 584 al., 2017). The richest horizon linked to the Rostamin tradition is AH III. The Bayesian OSL results for 585 sublayers IIIa, IIIb and IIIc suggest that the producers of Rostamian tradition likely occupied the site 586 of Ghār-e Boof between 37–39 ka (68% Cl). The obtain Bayesian chronology using both OSL ages and 587 <sup>14</sup> C dates resulted in 35–42 ka for AH III to AH IV (also sublayer IVa). Moreover, the result of 588 Bayesian modeling only for <sup>14</sup>C published in Becerra-Valdivia et al. (2017) yielded the age of 41,950– 589 39,850 cal BP (in 68% CI), which corresponds to the beginnings of the Upper Paleolithic period for 590 the site and for the Zagros as a whole. These results agree with the Bayesian OSL ages of the AH IV 591 and AH IVa of 40–42 ka.

592 Sublayers AH IVc and AH IVd have low find densities and cannot at present be attributed with 593 confidence to either the Middle or the Upper Paleolithic. Although Arjeneh point and perforated 594 shells were observed in AH IV to AH IVb, which we attribute to the Upper Paleolithic, they are 595 missing in AH IVc and AH IVd. As a result, the age of AH IVd 45–48 ka may be considered to 596 represent the period between Middle Paleolithic and the Rostamian at Ghār-e Boof.

597 In summary, the Bayesian OSL ages determined for the Upper Paleolithic sequence of the site 598 from AH IIIa to AH IVa resulted in ages of 37–42 ka (68% Cl). This range agrees with the chronology 599 for the Upper Paleolithic of the Shanidar cave in the north of Zagros which is in ca. 29-40 cal ka BP 600 (original data: Solecki 1963; Hole and Flannery, 1968; recalculated data: Becerra-Valdivia et al., 601 2017). This result is also in agreement with the Upper Paleolithic chronology provided for the site of 602 Yafteh associated with the Baradostian culture (Otte et al., 2011; ca. 29-42 cal ka BP). Aside from 603 the controversial ages for the early Upper Paleolithic of the Kaldar cave with the range of ca. 37–54 604 cal ka BP (Bazgir et al., 2017), the results from Ghār-e Boof are consistent with the Upper Paleolithic 605 chronology known elsewhere in the Zagros.

In general, the chronology for the Upper Paleolithic part of the site of Ghār-e Boof, like other sites mentioned in the Zagros Mountains, seems to be older than the chronology provided for the Paleolithic sites located in the north of central Iranian desert. For instance, the site of Garm roud 2, which is situated in the north of the Alborz Mountains region, suggests an Upper Paleolithic settlement between 28–35 cal ka BP (Berillon et al., 2007; Antoine et al., 2016). Moreover, the Bayesian OSL dating for the Upper Paleolithic sequence of the open-air site of Mirak (Vahdati Nasab et al., 2019) resulted in 21–28 ka (Heydari et al., 2020). 613 The Middle Paleolithic Bayesian OSL chronology from AH V starts with the age of 46–49 ka. 614 Below, AH Va in the western and the northern wall the Bayesian ages result in 51–55 ka and 55–58 615 ka. The age results for the sublayers of AH V, AH Vb and AH Vc encompass the range of 56–60 ka and 616 58–63 ka. The two Bayesian ages for the last layer AH VI from the top and the bottom exhibited 72– 617 78 ka and 75–81 ka. In summary, the chronology of the archaeological layers containing Middle 618 Paleolithic assemblages shows a wide range of 45-81 ka, starting with the range of 72-81 ka and 619 continuing to the very late Middle Paleolithic ca. 45 ka. The Middle Paleolithic deposits at Ghār-e 620 Boof (AH IVd - AH VI) are not as rich as the Rostamian part of the sequence. Although the Middle 621 Paleolithic assemblages have not yet been published in detail, we argue that there is no continuity is 622 observed between the Middle Paleolithic and the bladelet assemblages of the Upper Paleolithic at 623 Ghār-e Boof (Bretkze and Conard 2017; Conard and Zeidi 2019). The much lower density of the 624 Middle Paleolithic assemblages appears to reflect sporadic, short-term occupations characterized by 625 diverse scrapers and a dominance of flake production. These assemblages stand in stark contrast to 626 the rich unidirectional bladelet production during the Rostamian. Also the rich record of personal 627 ornaments, including numerous perforated shells and a perforated incisor of an ungulate (Conard and Ghasidian, 2011; Conard and Zeidi, 2019), is thus far limited to the Rostamian deposits. We 628 629 hypothesize that the Rostamian appeared due to the presence of a new group of AMH in the region. 630 This population was likely different from the humans who created the relatively sparse Middle 631 Paleolithic record from period preceding the Rostamian. For the moment, we do not know which 632 human species were responsible for Middle Paleolithic assemblages recovered from Ghār-e Boof. 633 This being said, to date, the evidence available from sites in the Zagros including Bisitun Cave, 634 Shanidar and Wezmeh suggest that Neanderthals were often responsible for making Middle 635 Paleolithic assemblages (Coon, 1951; Solecki, 1963; Trinkaus, 1983; Zanolli et al., 2019). On the other 636 hand, the complex record of human fossils dating to the Late Middle Pleistocene and Upper 637 Pleistocene in southwestern Asia as a whole points to a long history of early modern humans in the 638 macro-region and warns against rushing to hasty conclusions in the absence of human skeletal 639 remains (Hershkovitz et al., 2018).

640 In summary, our study shows that Ghār-e Boof was occupied intensely during MIS (Marine 641 Isotope Stage) 3 (after Lisiecki and Raymo, 2005) near the beginning of the Upper Paleolithic. The 642 site was occupied during MIS 3, MIS 4 and MIS 5a by the makers of the Middle Paleolithic assemblages. Although many questions remain open, it is worth mentioning that the new Middle 643 644 Paleolithic chronology for the site of Ghār-e Boof represents the first reliable absolute chronology 645 for the Middle Paleolithic of the southern Zagros. Due to the unique location of Ghār-e Boof, and the 646 likely association of the Rostamian with modern humans, our chronology provides insights into 647 dispersal routes of early modern humans from Africa toward central Asia through the south of the 648 Iranian Plateau. To decipher the full picture in the southern Zagros, more archaeological fieldwork 649 and paleochronological studies are needed in the future.

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### 651 **5.** Conclusions

652 We have presented a luminescence chronology based on quartz and the polymineral for the Middle and Upper sequences of the site of Ghār-e Boof. Our investigation showed that the pIRIR<sub>290</sub> 653 654 ages for the polymineral fractions are in good agreement with the blue-OSL ages of the quartz grains. Additionally, previously published <sup>14</sup>C ages for the Upper Paleolithic part of the cave agree 655 656 with the luminescence ages. We then applied Bayesian modeling, specifically designed for 657 luminescence dating on blue-OSL quartz signals using the R package 'BayLum', which enabled us to incorporate the published <sup>14</sup>C ages and well-established stratigraphic constraints to further improve 658 659 the precision of the chronology. The obtained Bayesian ages resulted in a significant improvement of 660 precision by reducing the age uncertainties. The Bayesian ages of the Upper Paleolithic sequence of 661 the cave for AH IIIa to IVa produced ages of 37–42 ka (68% CI). This result is in agreement with the chronology based on <sup>14</sup>C (Conard and Ghasidian 2011; Baines et al., 2014; Becerra-Valdivia et al., 662 663 2017).

664 The chronology obtained for the Middle Paleolithic sequence of the cave in AH IVd and AH VI 665 resulted in a wide age range of 45–81 ka (68% Cl). This work provides a solid luminescence-based 666 chronology for the Middle Paleolithic period in Iran. Moreover, the Bayesian OSL chronology for the site of Ghār-e Boof is the first complete luminescence dating of the Middle and the Upper Paleolithic 667 668 periods in the Zagros Mountain region in Iran. The radical change in material culture between the 669 Middle Paleolithic and Rostamian Upper Paleolithic occupations at Ghār-e Boof almost certainly 670 documents the occupation of the site by different groups of humans during MIS 3, MIS 4 and MIS 5a. 671 While we have good reasons to hypothesize that the Rostamian assemblages were left by AMH, 672 both Neanderthals and modern humans remain plausible candidates as the makers of the sites 673 Middle Paleolithic assemblages. Regardless of the specific identity of these populations, the 674 chronostratigraphic sequence from Ghār-e Boof points to a shift between the Middle Paleolithic and 675 Rostamian demographic groups within three millennia.

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954

# Figure captions Figure 1. a) Dasht-e Rostam region; the dashed areas show Dasht-e Rostam I and Dasht-e Rostam II, the site of Ghār-e Boof is located at the microhabitat of Yagheh Sangar. b) Location of the Paleolithic sites in the region, as mentioned in the text. c) Photo of the site of Ghār-e Boof. Figure 2. Synthetic stratigraphic sections of the western and northern walls of the site of Ghār-e Boof. Locations of the luminescence samples, as well as the <sup>14</sup>C dates published in Conard and

962 Ghasidian (2011), Baines et al. (2014) and Becerra-Valdivia et al. (2017) are shown.

963

Figure 3. TL curves, shine-down curves and typical dose-response curves of samples GB1 for both
 quartz (a) and polymineral fractions (b). Abbreviations: TL = thermoluminescence; OSL= optically
 stimulated luminescence; IRSL= infrared stimulated luminescence.

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**Figure 4.** Distribution of equivalent doses of samples GB3 and GB14 as examples from the quartz (a, b) and polymineral fractions (c, d). The final equivalent doses are determined based on arithmetic average, and the uncertainty is estimated according to the standard error of the mean. Abbreviations:  $D_e$  = equivalent dose; *n* = number of aliquots; abs. se = absolute standard error.

972

973 Figure 5. Radioactive disequilibrium check for the <sup>238</sup>U decay chain. The ratios of <sup>238</sup>U (post-<sup>226</sup>Ra)/<sup>232</sup>Th and <sup>238</sup>U (pre-<sup>226</sup>Ra)/<sup>232</sup>Th for the entire samples are shown. Most of the samples lie <sup>975</sup> close to the equilibrium line except for samples GB2, GB4, GB7, GB10, GB13, and GB14 (they are <sup>976</sup> color-coded in red). For these samples, averages of the top (pre-<sup>226</sup>Ra) and the bottom (post-<sup>226</sup>Ra) of <sup>977</sup> the <sup>238</sup>U decay chain were used to determine the dose rates.

978

979 Figure 6. Results of the quartz OSL ages and pIRIRSL<sub>290</sub> ages of the polymineral fractions within 68 %
980 confidence interval. The quartz and polymineral ages overlap one another, and they gradually

981 increase with depth. The <sup>14</sup>C ages (2014) are taken from Conard and Ghasidian (2011) and Baines et
982 al. (2014), while the <sup>14</sup>C ages (2017) are taken from Becerra-Valdivia et al. (2017). Abbreviations:
983 OSL= optically stimulated luminescence; pIRIRSL<sub>290</sub> = post-infrared infrared stimulated luminescence
984 at 290 °C.

985

**Figure 7.** Ages obtained after incorporating the Bayesian OSL (optically stimulated luminescence) ages with the calibrated <sup>14</sup>C dates published in Conard and Ghasidian (2011), Baines et al. (2014), and Becerra-Valdivia et al.(2017) using the R package 'BayLum'. The Bayesian model addresses the shared systematic error between samples, and it also includes stratigraphic constraints.

990

**Figure 8.** Comparison of the OSL (optically stimulated luminescence) Bayesian quartz ages with the ages derived from the classical approach. As illusterated applying stratigraphic constraints and incorporating the <sup>14</sup>C dates play a fundamental role in reducing the uncertainties at the top of the age sequence. However, even at the bottom where age intervals overlap with one another, the Bayesian uncertainties are smaller than the corresponding classical approach. 51°12′E

9

m

30°

30°24'N

30°1

51°24′E



51°36′E













10

15

Precision

20

25

0.031

Density (bw 0.053)

n = 30 | in 2 sigma = 80 % | mean = 103.52 | abs. se = 2.66





0.066

Density (bw 0.042)

b

5

10

15

Precision

20

25

а





# Bayes estimator C14Cal1(III) 68% credible interval C14Cal2(III) 95% credible interval GB1(IIIa) GB2(IIIb) C14Cal3(IIIb) C14Cal4(IIIb) GB3(IIIc) C14Cal5(IV) C14Cal6(IV) GB4(IV) GB5(IVa) C14Cal7(IVa) GB6(IVd) GB7(V) GB8(Va) GB9(Va) GB10(Vb) GB11(Vc) GB13(VI) GB14(VI) 40 50 60 70 80

# Ages results

Age (ka)



# Table 1

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The radionuclide concentration derived by gamma-ray spectrometry.

Sample name	K (%)	σ	U pre-Ra (ppm)	σ	U post-Ra (ppm)	σ	Th (ppm)	σ
GB1	1.01	0.02	1.51	0.11	1.33	0.03	2.80	0.06
GB2	0.84	0.02	1.49	0.10	1.23	0.03	2.49	0.06
GB3	0.84	0.02	1.66	0.09	1.68	0.03	2.58	0.05
GB4	0.73	0.02	2.30	0.10	1.64	0.03	2.54	0.06
GB5	0.75	0.02	2.23	0.11	2.01	0.03	2.47	0.06
GB6	0.61	0.02	1.96	0.10	1.89	0.03	2.47	0.05
GB7	0.61	0.02	2.48	0.11	1.30	0.03	2.19	0.06
GB8	0.59	0.02	2.08	0.09	1.95	0.03	2.26	0.05
GB9	0.56	0.02	2.26	0.10	2.06	0.03	2.24	0.05
GB10	0.62	0.02	2.43	0.10	1.82	0.03	2.31	0.05
GB11	0.49	0.01	2.24	0.09	2.15	0.03	1.96	0.04
GB12	0.38	0.01	2.13	0.09	2.06	0.03	1.68	0.04
GB13	0.40	0.01	2.59	0.09	1.99	0.03	1.70	0.04
GB14	0.64	0.02	2.89	0.12	2.44	0.04	2.58	0.06

Abbreviation:  $\sigma$  = error-propagated uncertainty.

# Table 2

## The determined environmental dose rates.

Sample name	Alpha-D <sub>r</sub> (Q) (Gy/ka)	σ	Alpha-D <sub>r</sub> (PM) (Gy/ka)	σ	Beta-D <sub>r</sub> (Gy/ka)	σ	Gamma-D <sub>r</sub> (Gy/ka)	σ	In situ gamma-D <sub>r</sub> (Gy/ka)	σ	Cosmic-D <sub>r</sub> (Gy/ka)	σ	Total-D <sub>r</sub> (Q) (Gy/ka)	σ	Total-D <sub>r</sub> (PM) (Gy/ka)	σ
GB1	0.04	0.01	0.14	0.02	0.89	0.05	0.46	0.02	0.49	0.03	0.11	0.01	1.55	0.06	1.81	0.07
GB2	0.04	0.01	0.13	0.02	0.77	0.04	0.41	0.02	0.42	0.02	0.10	0.01	1.34	0.04	1.60	0.06
GB3	0.05	0.01	0.15	0.02	0.80	0.04	0.44	0.02	0.44	0.02	0.10	0.01	1.40	0.04	1.67	0.06
GB4	0.05	0.01	0.17	0.02	0.77	0.04	0.45	0.02	0.46	0.01	0.10	0.01	1.39	0.04	1.67	0.06
GB5	0.06	0.01	0.17	0.03	0.80	0.04	0.45	0.02	0.46	0.02	0.10	0.01	1.42	0.04	1.71	0.06
GB6	0.05	0.01	0.16	0.02	0.68	0.03	0.41	0.01	0.43	0.01	0.09	0.01	1.26	0.03	1.54	0.06
GB7	0.05	0.01	0.15	0.02	0.67	0.03	0.40	0.02	0.40	0.03	0.09	0.01	1.23	0.05	1.50	0.07
GB8	0.05	0.01	0.16	0.02	0.67	0.03	0.40	0.01	0.42	0.01	0.09	0.01	1.24	0.03	1.52	0.06
GB9	0.05	0.01	0.17	0.03	0.67	0.03	0.41	0.02	0.40	0.03	0.09	0.01	1.22	0.05	1.51	0.07
GB10	0.05	0.01	0.17	0.03	0.71	0.03	0.43	0.02			0.08	0.01	1.25	0.05	1.57	0.06
GB11	0.05	0.01	0.17	0.03	0.62	0.03	0.39	0.01			0.08	0.01	1.16	0.04	1.43	0.06
GB12	0.05	0.01	0.16	0.03	0.53	0.02	0.35	0.01			0.08	0.01	1.02	0.03	1.29	0.05
GB13	0.05	0.01	0.16	0.03	0.54	0.03	0.36	0.02			0.08	0.01	1.04	0.04	1.31	0.06
GB14	0.06	0.01	0.20	0.03	0.75	0.04	0.47	0.02			0.08	0.01	1.38	0.05	1.68	0.07

Abbreviations: Q = quartz; PM = polymineral;  $\sigma$  = error propagated uncertainty; D<sub>r</sub> = estimated dose-rate.

# Table 3

Sample	D <sub>e</sub> (Q)	6514		_	D <sub>e</sub> (PM)	6514	Age (PM)	_
name	(Gy)	SEIVI	Age (Q) (ka)	σ	(Gy)	SEIVI	(ка)	σ
GB1	59	1	38	2	68	1	37	2
GB2	55	1	42	2	65	1	41	2
GB3	55	1	39	2	69	2	42	2
GB4	55	1	40	2	65	2	39	2
GB5	55	1	39	2	68	2	40	2
GB6	60	1	48	2	71	2	46	2
GB7	55	1	45	2	67	2	45	2
GB8	65	2	52	2	88	4	58	3
GB9	74	2	61	3	90	3	60	4
GB10	70	1	56	3	88	3	56	3
GB11	69	1	59	3	87	5	60	4
GB12	-	-	-	-	86	2	66	3
GB13	80	2	77	4	102	4	77	5
GB14	104	3	76	4	124	3	74	4

The equivalent dose and corresponding ages in the classical approach.

Abbreviations:  $D_e$  = equivalent dose; SEM = standard error of the mean;  $\sigma$  = error propagated

uncertainty; Q = quartz; PM = polymineral.