

Reconciling the contradicting results from computational and experimental studies of high-pressure minerals

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Recently, the great success of *ab initio* simulation has contributed to improve our understanding of the inner Earth's dynamics. In contrast, high-P experiments have also provided valuable data. The combination of different scientific perspectives is necessary for the development of a consistent model of the Earth's mantle and core. However, some results from *ab initio* computations contradict those from high-P experiments. In order to reconcile these issues, we have performed both DFT computations and synchrotron high-P experiments. VASP code and diamond anvil cell were used for *ab initio* computations and high-P experiments, respectively. In this talk, three issues (magnesium-aluminium oxide, carbonate, and iron carbide) will be presented. In the case of magnesium-aluminium oxide (MgAl_2O_4), previous computational study [1] could not explain the pressure-induced transition sequence observed in high-P experiments. Our experimental [2] and computational [3] studies showed that previous computational study had a significant uncertainty for comparing energetics of different structures, because of a lack of the relaxation of atoms. In the case of carbonate (CaCO_3), a new mineral predicted by *ab initio* simulations [4] could be synthesized by diamond anvil cell experiments [5]. The new high-P phase of carbonate has a four-fold coordination of carbon cations. In the case of iron carbide (Fe_3C), the magnetic transition pressure is inconsistent (5–70 GPa) among previous experimental studies. In contrast, *ab initio* simulations predicted that the magnetic transition occurs at ~60 GPa [6]. Our results from both high-P experiments and *ab initio* simulations showed the transition pressure was ~55 GPa. This indicated that previous experiments have a large uncertainty for the detection of the change in magnetic properties of iron carbide.

[1] Gracia *et al.* (2002) *Phys. Rev. B* **66**, 224114. [2] Ono *et al.* (2006) *Phys. Chem. Minerals* **33**, 200. [3] Ono *et al.* (2008) *Phys. Chem. Minerals* **35**, 381. [4] Oganov *et al.* (2006) *Earth Planet. Sci. Lett.* **241**, 95. [5] Ono *et al.* (2007) *Am. Mineral.* **92**, 1246. [6] Vočadlo *et al.* (2002) *Earth Planet. Sci. Lett.* **203**, 567.

A provenance study of marbles from the Roman town of Thamusida (Mauretania Tingitana, northern Morocco)

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A combined mineralogical and geochemical approach is being used to determine the provenance of the white and coloured marbles found in the archaeological site of *Thamusida* in Mauretania Tingitana Roman province, northern Morocco. Of particular interest is to assess the exploitation and use of local raw material that mostly consists of limestone and metamorphic marble of the coastal Paleozoic basement. 75 samples from ancient and modern quarries, covering as many different lithotypes as possible, were compared with 26 fragments from archaeological artefacts. Both sample sets were submitted to petrographic and mineralogical studies, using OM, SEM, and XRD. The geochemical analyses include major and trace elements and stable C and O isotope compositions.

The archaeological samples made of crinoidal grainstone ($\delta^{13}\text{C}$: 0.4 and 0.7‰, $\delta^{18}\text{O}$: -5.3 and -3.9‰ VPDB) and the one made of packstone ($\delta^{13}\text{C}$: 1.8 and $\delta^{18}\text{O}$: -7.3‰) fall within the ranges ($\delta^{13}\text{C}$: 0.2 to 2.2‰, $\delta^{18}\text{O}$: -3.1 to -5.8‰ and $\delta^{13}\text{C}$: 0.2 to 2.4‰ to $\delta^{18}\text{O}$: -5.1 to -10.8‰) defined for the quarries located in the Tiflet-Sehoul zone (SE Rabat). The local white marbles have an isotopic composition ($\delta^{13}\text{C}$: -2.0 to 2.4‰, $\delta^{18}\text{O}$: -15.8 to -7.8‰, n= 28) significantly different to that of the white marble artefacts ($\delta^{13}\text{C}$: -0.9 to 3.5‰, $\delta^{18}\text{O}$: -8.1 to -1.6‰, n= 21). This data indicate that Moroccan material can be excluded as source of the studied white marble artefacts. The comparison with published database on Mediterranean marbles allowed identifying some other provenances, such as Carrara marble for a 'Togato' statue ($\delta^{13}\text{C}$: 2.2‰ and $\delta^{18}\text{O}$: -1.7‰). The results of this work give for the very first time a detailed characterization of local stone material from the area of *Thamusida*. The stable isotope data point clearly to the provenance of some artefacts, particularly those made from coloured limestones.