New constraints on Xe incorporation mechanisms in olivine from First-principles calculations

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Storage of Xe at depth in silicate minerals has recently been proposed to explain the low Xe abundance in the Earth's and Mars' atmospheres compared to other noble gases [1]. Evidences for incorporation of Xe in olivine, at pressure and temperature relevant for the lithosphere, are based on observed variations in cell parameters and the appearance of a new Raman band [2]. We perform calculations using density functional theory and found that only Xe for Si substitution is able to reproduce all experimental observations. An estimation of Xe content in Xe-rich olivine, based on present work and previous *in situ* experimental results [2], shows that up to 0.4 at% Xe could be stored in olivine at depth. Using this value and Xe solubility of tholeitic melt from [3] we found a melt-partitioning coefficient of 5 (at ~ 1 GPa and 1500 K), challenging the supposedly incompatible behavior of Xe in olivine.

[1] Anders and Owen (1977) *Science* **198**, 453-465. [2] Sanloup et al. (2011) *Geochim. Cosmochim. Acta* **75**, 6271–6284. [3] Schmidt and Keppler (2002) *EPSL* **195**, 277-290.