Postdoctoral Position in Computational Molecular Modelling for Geochemical Applications

A post-doctoral position is available at the IMPMC laboratory (Université Paris VI, France, http://www.impmc.upmc.fr). It is a full-time position for two years, funded by the ANR (The French National Research Agency).

The proposing group is one of the world-leading groups in the field of the theoretical determination of isotopic properties of a system from *ab initio* calculation of the vibrational density of states. The method has been successfully applied to solids (e.g. Blanchard et al. 2009). The post-doctoral fellowship will be mainly devoted to the development of this method to liquid phases. This work will be conducted within a collaborative project involving mineralogists and physicists, which aims at improving our understanding of the crystal-chemistry of iron-bearing minerals and of the geochemistry of minor and trace metal pollutants at solid-solution interfaces.

Applicants should have a strong background in quantum molecular computer simulations (computer codes employed in this project are based on density functional theory). Knowledge in geosciences will be greatly appreciated. For further information, please contact:

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Applications, including a detailed CV, a list of publications and a short summary of research activities should be sent to marc.blanchard@impmc.upmc.fr

Reference

Blanchard M., Poitrasson F., Méheut M., Lazzeri M., Mauri F. & Balan E. (2009) Iron isotope fractionation between pyrite (FeS_2), hematite (Fe_2O_3) and siderite ($FeCO_3$): A first-principles density functional theory study, *Geochim. Cosmochim. Acta*, **73**, 6565-6578