A one-year postdoc position (with possible extension for another year) is opened in the joint CNRS/MIT "MultiScale Materials Science for Energy and Environment" research group led by Dr. Roland Pellenq and Prof. Franz J. Ulm to work on the prediction of Raman spectroscopic properties of disordered carbonaceous systems from computer simulations. The target materials of the project are both immature (essentially aliphatic) and mature (aromatic) kerogens, the organic inclusions present in shale rocks.

The hired candidate will be located on the MIT campus in Cambridge Massachusetts (although some extended stays in Bordeaux, France, are expected). He will work in a first step under the supervision of Dr Jean-Marc Leyssale on the development on atomistic models of disordered carbons, using Reverse Monte Carlo and molecular dynamics techniques, and on the prediction of their non-resonant Raman spectra using classical and *ab initio* molecular dynamics. Expected outcomes are the correlations between the structure of the materials and the width of their Raman G band [1].

He will then collaborate with Dr. Lionel Truflandier from the University of Bordeaux, Institute of Molecular Sciences (France) with the support of Pr. David R. Bowler University College London (London Centre for Nanotechnology), in implementing and testing non-resonant/resonant Raman intensity calculation[2] using a density-functional theory based tight-binding approach as implemented in the CONQUEST code.[3] This will be applied to the prediction of the full Raman spectra of carbon models, focusing especially on the defect-induced Raman D band as observed in disordered graphitic materials[4]

Candidates should have a solid background in quantum electronic structure theory with good knowledge in numerical sciences. Good communication skills in English are mandatory. Previous experiences with (either) condensed matter theory, density functional theory, and LINUX environment/scientific programming are required. Some experience with disordered/amorphous systems would also be welcome.

Applications should include a detailed CV, a brief description of motivations, and the contact information of at least two referees. Inquiries and applications should be sent to Jean-Marc Leyssale (leyssale@mit.edu) and Lionel Truflandier (l.truflandier@ism.u-bordeaux.fr) Consideration of candidates will begin immediately and continue until the position is filled. The net monthly salary will be of 2,900 €.

[1] Romero-Sarmiento M.-F., Rouzaud J.-N., Bernard S., Deldicque D., Thomas M., Littke R., *Org. Geochem.* **2014,** *71*, 7-16.
[2] See, e.g. Profeta M., Mauri F., *Phys. Rev. B* **2001**, *63*, 245415.
[3] http://www.order-n.org; D. R. Bowler and T. Miyazaki, D. R. Bowler and T. Miyazaki, *J. Phys.: Condens. Matter* 22, 074207 (2010).
[4] Ferrari A. C., Robertson J., *Phil. Trans. R. Soc. Lond. A* **2004**, *362*, 2477-2512.

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