



Postdoc position in Condensed Matter Theory  
CNRS and Sorbonne Université, Paris, France

**Accurate determination of infrared spectroscopy  
in hydrogen-rich materials**

We offer a postdoc position at Sorbonne University in Paris, under the supervision of M. Casula and R. Vuilleumier. We aim to extend the molecular dynamics (MD) coupled to quantum Monte Carlo (QMC) calculations, in order to compute the vibrational properties of hydrogen-rich systems, where nuclear quantum effects are relevant. This class of systems includes the latest synthetized compounds that are superconductors with record breaking critical temperatures. The postdoctoral researcher will carry out first-principles and analytical calculations to study these compounds, by using advanced QMC and MD methods. She/he will develop new numerical approaches to compute their vibrational properties.

The fellowship, funded by the Sorbonne Excellence Cluster "MATISSE" (MAterials, InterfaceS, Surfaces, Environment), should start at the earliest convenience, will last up to 18 months, and has to be filled by July 2019. It includes resources to support participation to conferences and visiting stays. The net salary starts from around 2100€ depending on the candidate work experience. The postdoctoral fellow will join the group "Théorie Quantique des Matériaux" at the Institut de Minéralogie, de Physique des Matériaux et de Cosmochimie (IMPMC UMR 7590), and work in collaboration with the Chemistry Department (theoretical chemistry group, UMR 8640 PASTEUR) at the École Normale Supérieure, Paris.

The ideal candidate should have a solid background in condensed matter physics and a good experience in electronic structure calculations. She/he should have worked with QMC and MD methods and possibly should be a developer of existing QMC/DFT/MD codes. Experience in methodological developments of first-principles approaches is highly appreciated.

If you are interested, please apply electronically (join a CV including full publication list and arrange for three reference letters) by sending an e-mail to:

michele.casula@gmail.com

rodolphe.vuilleumier@ens.fr

A decision will be taken most likely by late April 2019.

For full publication list, see:

<http://www.researcherid.com/rid/B-4110-2016>

<https://orcid.org/0000-0001-5386-699X>