

Post-doc opportunity at CentraleSupélec (former Ecole Centrale Paris, France) in Numerical Method for Quantum Chemistry and Physics.

The Laboratory "Structure, Properties and Modeling of Solids Modeling" is a joint research unit between the Ecole Centrale Paris and CNRS. One of our goals is to discover materials of the future in key areas such as energy, electronics and health. Our strength is to work both on the exploration of new compounds, new developments, but also on the characterization of advanced structural and functional properties of produced materials. Another important objective is to develop new investigation tools for a better experimental and theoretical understanding of matter from a sub-atomic scale up to a scale of several hundred microns. Our laboratory is at the border between chemistry and physics, so it naturally develops an interdisciplinary approach. SPMS laboratory enjoys a leading academic setting within the CentraleSupélec engineering school in the University Paris Saclay.

Partial description of our activities can be found at

http://www.ecp.fr/cms/lang/en/Research/Laboratories/SPMS_1

Within SPMS lab, our group is active in modelling electron densities and electron density properties in molecules and crystals either by means of ab initio computing methods (Gaussian09 or CRYSTAL14 code) or by refinement of quantum theoretical models against experimental X-ray and neutron scattering data. Other experimental methods are also considered.

We offer a 12 to 18 months post-doc position to help develop new efficient means to reconstruct a One electron Reduced Density Matrix from experimental data. The candidate is expected to master efficient computer coding (Fortran, C++) together with knowledge of numerical methods adapted to quantum chemistry. He would ideally hold a PhD degree in applied mathematics, theoretical physics or chemistry.

Please send application with a CV and recommendation letter to:

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Surface mail:

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