ÉCOLE DOCTORALE
SCIENCES DE LA TERRE ET DE L'ENVIRONNEMENT
ET PHYSIQUE DE L'UNIVERS, PARIS

Subject offered for a contract starting october 2015

SUBJECT TITTLE: Core Composition and Stratification form FPMD Calculations

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Host lab/ Team : *please fill in and leave out meaningless information*
IPGP - Géophysique Expérimentale – UMR 7154

Financing: Doctoral contract with or without assignment

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Presentation of the subject: (1 or 2 pages)

The composition of Earth's core is an essential yet still open question in the geological sciences. From the analysis of iron meteorites, the observation of Earth's moment of inertia, and from seismic normal mode studies, we know that the primary constituent is an iron (Fe) alloy with ~4.5% nickel (Ni) and a suite of siderophile trace elements. Normal-mode studies provide a good density profile of the entire core; comparing the observed density with the experimentally measured one led Birch to propose that the density of the core is less than that of pure iron. Shockwave and static diamond anvil cell (DAC) experiments have further estimated the deficit to be between 5 and 10%. To account for that, lower atomic weight elements have been suggested as additional constituents. Moreover, the density jump at the inner core boundary (ICB) between the solid inner core and liquid outer core is about 4.5%, too large to be due just to the phase transition, and indicates that the outer core contains more light elements (~5 to 10%) than the inner core (~2 to 3%). The prime light-element candidates for the core, taking into account cosmochemical and petrological constraints, are silicon, sulphur, carbon, and oxygen. Models for core composition allow *in principio* a mixture of several light elements, and many arguments have been put forward over the years for and against each of the elements.

In order to constrain the very wide range of possible light-element compositions in the core, we propose to calculate the density and bulk sound velocity of Fe-Ni-C-O-Si-S liquid alloys using *ab initio* molecular dynamics. The advantage of this is that we can then compare possible light-element compositions directly with the primary geophysical observations (*e.g.* density and bulk sound velocity obtained from radial seismic models). The calculations will be performed on liquid iron, alloyed with various elements (C, O, Si, S, and Ni) in the pressure and temperature range of the outer core (135-330 GPa, 4300-6300 K). The FP molecular dynamics simulations will be carried out using DFT with the VASP code, which incorporates the projected augmented wave (PAW) method to represent the electron orbitals and two approximations to DFT: GGA and LDA.