OPEN POSTDOCTORAL POSITION

Title Thermodynamics and dynamics of carbon/iron clusters: a theoretical approach to modeling the growth of carbon nanotubes.

Location Laboratoire Francis Perrin (LFP) CEA-CNRS URA 2453
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Funding program, salary, duration C2EA is a French organization centered on fundamental and applied research in alternative and nuclear energies. The postdoctoral position is funded ASAP for **12 months** by its national program "*Nano-simulation*". The salary will be that of a staff C2EA agent of equivalent qualifications to that of the postdoctoral applicant.

The research group: The "Reaction Dynamics" group at LFP is specialized in fundamental chemical physics, specifically to the detailed understanding of the dynamics of chemical reactions when chemical bonds rearrange. It has initiated a long term research project for simulating the growth of carbon nanotubes on iron clusters, in line with the activity of the "Nanometric Structure" group at LFP.

Job description: The project has two directions, which will be developed by the prospective applicant in strong connection with two staff scientists of C2EA (C. Angelié and J.-M. Soudan) and a PhD student (opened position).

The first direction is already under progress. It concerns the thermodynamics of iron/carbon clusters. The original Metropolis algorithm and the Wang-Landau method have been associated in a new Monte-Carlo scheme to get state densities of which thermodynamic properties are deduced. This will be applied to the fusion or vaporization of iron/carbon clusters with low carbon content, which are confined either by a fixed wall or within an elastic carbon nanotube. A medium level reactive potential (MEAM) is used for this direction. The second direction of the project aims at simulating the growth of carbon nanotubes on iron clusters by extensive molecular dynamics calculations (simulated time$\sim$1 ns; $\sim$1000 atoms). Realistic high level empirical potentials of the reactive type will be implemented for this purpose by a combination of two potentials grounded on the Tight Binding method.

Key words: Modeling, iron/carbon cluster, Monte-Carlo, molecular dynamics

Required qualifications We are seeking a post-doc with documented skills in molecular dynamics and Monte Carlo simulations. The applicant should be used to work with and also to modify heavy computer codes. Knowledge of reactive potentials and of the Tight Binding method is wished. The post-doc will have the main responsibility of the project direction on nanotube growth.

Application procedure The application shall be written in English or French and include the following items:

1. A description of the qualification for the position
2. Curriculum Vitae including a list of publications
3. Two reference persons who can be contacted (describe the association with them and give the contact addresses)