Ecole Doctorale des Sciences Chimiques ED250

Contrats Doctoraux **2016**

Title :

Development of molecular pseudopotentials for the study of properties and chemical reactions in condensed phase.

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Project :

This theoretical chemistry project aims to simplify the study of experiences made in rare-gas matrices for reproducing interstellar conditions.
From a computational point of view, the description of the environment (i.e. the rare-gas matrix) is resource-consuming. Within the CTOM group, pseudopotentials have been already developed to treat the environment of chemical systems by reducing the computational cost. We propose to further develop those methods and to adapt them to reproduce effects of more complex chemical means, such as the gas-rare matrices. This project will imply some programming (Fortran and/or python).

Context :

This study continues efforts on pseudopotential development of the CTOM group, as well as current and established joint work with experimentalists on systems in matrices. [1,2]

References:

[1] J. Drujon and Y. Carissan, *Journal of Computational Chemistry*, 2013, **34**, 49–59.

[2] T. Butscher, F. Duvernay, P. Theule, G. Danger, Y. Carissan, D. Hagebaum-Reignier, and T. Chiavassa *MNRAS*, 2015, **453**, 1587-1596.