Namur Institute of Structured Matter

UNIVERSITÉ DE NAMUR

NISM Seminar

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« CRYSTAL and CRYSCOR: two modern tools for the *ab initio* study of crystalline solids. Recent developments and perspectives. »

When and where:

Thursday October 3rd 2019 at 16:00
UNamur, Rue Grafé 2, B-5000 Namur
Chemistry & Physics building
Auditorium CH21 (2nd floor)

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« CRYSTAL and CRYSCOR: two modern tools for the *ab initio* study of crystalline solids. Recent developments and perspectives. »

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The CRYSTAL program [1] has been developed since the 1970s and is one of the most widely used softwares for the quantum-mechanical study of crystalline solids. It allows to compute the electronic structure of periodic systems within Hartree Fock, density functional or various hybrid approximations (global, range-separated and double-hybrids).

The Bloch functions of the periodic systems are expanded as linear combinations of atom centred Gaussian functions. As a consequence, global and range-separated hybrid functionals are accessible at a moderate computational cost.

CRYSTAL automatically handles space symmetry and allows calculation for system periodic in 3D (bulk), 2D(slabs), 1D(polymers) or, as a limiting case, 0D (molecule/cluster).

In the contribution I will present some of the most recent developments, including new tools for handling extended basis sets [2,3].

CRYSCOR [4] is a post-HF program able to efficiently compute the MP2 energy correction for crystalline solids on top of the CRYSTAL Harteee-Fock solution. CRYSCOR adopts a local approach [5], combined with an efficient parallelization [6] and the use of Orbital-Specific Virtuals [7] for the automatic definition of a truncated virtual space. I will present some recent application of the method, including a recent study dealing with crystal structure prediction of Copper (I) fluoride crystals.[8]

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[2] L. Maschio, B. Kirtman, *submitted*
[3] L. E. Daga, B. Civalleri, L. Maschio, *submitted*
[4] C. Pisani, L. Maschio, S. Casassa, M. Halo, M. Schütz, D. Usvyat, *J. Comp. Chem* **29** (2008) 2113.
[5] P. Pulay, Chem. Phys. Lett. **100**,151 (1983)
[6] L. Maschio, *J. Chem. Theory Comput*. **7**, 2818 (2011).
[7] D. Usvyat, L. Maschio, M. Schütz *J. Chem. Phys.* **143**(10), 102805 (2015)
[8] M. Kuklin, L. Maschio, D. Usvyat, F. Kraus, A. J. Karttunen *Chemistry - A European Journal* (2019)