Minicolloque n°4 ☒ **Oral** ☐ **Poster**

Experimental probe of the non-bonded interaction potential in endofullerenes: ^{3}He@C_{60} study

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Endofullerenes are supramolecular complexes consisting of a small (endohedral) atom/molecule enclosed by a fullerene (C60) cage[1,2]. Endofullerenes offer experimentalists with the molecular realisation of the ideal particle-in-a-box model, which enables one to directly observe translational (atomic) quantisation. The resulting energy diagram is sensitive to the intermolecular interaction potential. The aim of this study is firstly to observe transitions arising purely from atomic translational quantization due to confinement of a helium atom inside an almost spherical cage. Secondly, one aims at obtaining a detailed characterisation of the translational energy levels in an enlarged energy scale in order to derive experimentally the confining potential for the He@C60 complex. In this talk, it will show that from both terahertz IR spectroscopy coupled to neutron spectroscopy data, one can obtain information about the potential function V(r) representing the non-bonded interaction between the He atom and the C_{60} cage. Mainly showing it to be a superposition of r^2, r^4, and r^6 terms, which in turn can be tested against different theoretical models. Experiments of this kind provide high-quality experimental benchmarks for quantum chemistry calculations of non-bonded intermolecular and interatomic interactions.

[1] Levitt MH. 2013Spectroscopy of light-moleculeendofullerenes. Phil Trans R Soc A 371:20120429.
[2] K. S. K. Goh, M. Jimenez-Ruiz, M. R. Johnson, S. Rols, J. Ollivier, M. S. Denning, S. Mamone, M.H.Levitt, X. Lei, Y. Li, N. J. Turro, Y. Murata and A. J. Horsewill,Phys. Chem. Chem. Phys.,2014,16,21330-21339.

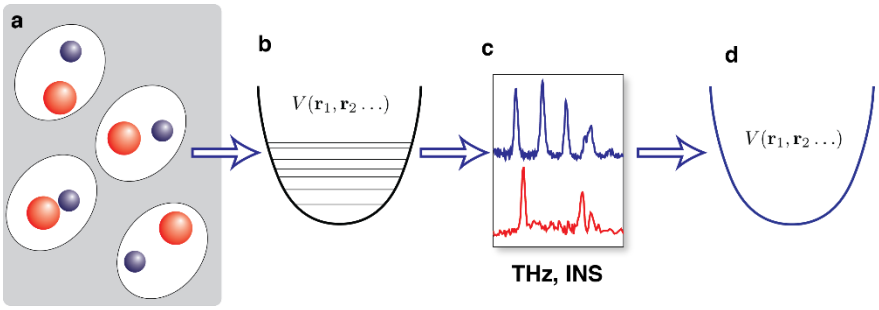

Figure 1: Analysis of the spectroscopic data allows determination of the potential energy function of the atom trapped in the C_{60}