Theoretical and Physical Chemistry Institute

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LECTURE

"On the Importance of Dynamics in Molecular Systems: From the Study of Nanostructure Formation to the Design of Photoactive Molecules"

Prof. Stefan Irle

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Friday, March 18, 2016, 12:00

Seminar room, ground floor, NHRF

On the Importance of Dynamics in Molecular Systems: From the Study of Nanostructure Formation to the Design of Photoactive Molecules

Stephan Irle

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Our group has successfully used the method of “direct quantum chemical molecular dynamics” (QM/MD) for the study of fullerene, carbon nanotube and graphene formation mechanisms. Key finding in our studies was that fullerene and initial stages of carbon nanotube and graphene formations are governed by kinetics, whereas the growth of nanotube sidewall and large areas of graphene follow thermodynamic principles.

Concerning the study of fluorescent dye molecules, we employed time-dependent density-functional tight-binding (TD-DFTB) and time-dependent density functional theory (TD-DFT) to understand the origin of the enigmatic blueshift in [n]cycloparaphenylene ([n]CPP) fluorescence, and the role of static and dynamic geometrical distortions in the bright states. QM/MD simulations performed on the excited state potential surfaces are able to explain the experimentally observed fluorescence blueshift of the strongest emission peaks with increasing molecular size. This unusual feature turns out to be a consequence of large vibrational amplitudes in small [n]CPPs, causing greater Stokes shifts, while large [n]CPPs are more rigid and therefore feature smaller Stokes shifts (“dynamic blueshift”) [2].

[1] S. Irle, A. J. Page, B. Saha, Y. Wang, K. R. S. Chandrakumar, Y. Nishimoto, H.-J. Qian, K. Morokuma, in: “Practical Aspects of Computational Chemistry II: An Overview of the Last Two Decades and Current Trends”, eds. J. Leszczynski and M. K. Shukla, Springer-European Academy of Sciences (2012).

[2] C. Camacho, Th. A. Niehaus, K. Itami, S. Irle, Chem. Sci. 4, 187 (2013).