Intra-cage Dynamics in Endohedral Fullerenes

–

Insight by Molecular Dynamics Simulations

K. Vietze and G. Seifert

Technische Universität Dresden
Institut f. Physikalische Chemie
Mommsenstr. 13
D-01069 Dresden
Germany

Intra-cage dynamics in endohedral fullerenes can reach a high degree of complexity ranging from anharmonic oscillations to fluxionality of the system, rendering experimental structural investigations and interpretations of spectroscopic data problematic. Common experimental techniques like NMR, EPR or IR/Raman only cover their own respective temporal regime and are bound to specific time scales. Hence, depending on the particular internal motion inside the carbon cage, these techniques probe only for specific aspects of the dynamics, e.g. short time snapshots or long term averages, resulting in possibly oppositional descriptions of the system. Especially the determination of molecular symmetries depends clearly from the spectroscopic method applied.

Molecular dynamics (MD) simulations within a Density Functional (DFT) based framework provide a detailed insight into the intra-cage dynamics and aid to clarify the dynamic behaviour whithin different time scales and its impact on spectroscopic investigations. This includes the description of structural transitions and the respective dynamic barriers, as well as the calculation of dynamic spectra of systems where the common harmonic approximation is insufficient.

Typical representatives of those species that were studied in detail include $Eu@C_{74}$, $Sc_3N@C_{80}$ and $Sc_2C_2@C_{84}$, which are characteristic examples for the complexity of the intra-cage dynamics and which illustrate the importance of a proper knowledge of these dynamics in order to find consistent interpretations of spectroscopic data.

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Presenting Author:
Vietze, K.
Technische Universität Dresden

Society Member: Yes ☐ No ☒

Complete Author List:

K. Vietze
Phone: +49(0)351-463 34648
Fax: +49(0)351-463 35953
E-Mail: Knut.Vietze@chemie.tu-dresden.de

G. Seifert
Phone: +49(0)351-463 37637
Fax: +49(0)351-463 35953
E-Mail: Gotthard.Seifert@chemie.tu-dresden.de

Technische Universität Dresden
Institut f. Physikalische Chemie
Mommsenstr. 13
D-01069 Dresden
Germany

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