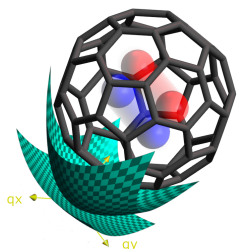


NON-ADIABATIC COUPLING IN NO@C₆₀: PREDICTION OF A RENNER-TELLER LIKE EFFECT FOR SPHERICALLY ENCAPSULATED DIATOMIC MOLECULES

ANDREAS W. HAUSER, JOHANN V. POTOTSCHNIG, *Institute of Experimental Physics, Graz University of Technology, Graz, Austria.*



The Renner-Teller effect describes the coupling of a symmetry-reducing molecular vibration with a two-fold degenerate electronic state. Its discovery goes back to work of Herzberg and Teller, who realized in 1933 that the potential energy surface of a triatomic, linear molecule splits into two as soon as the molecule is bent. In this work, we show that a very similar, yet unknown type of non-adiabatic coupling can even occur for diatomic (!) molecules.

This seems absurd at first sight, but becomes possible as soon as the diatomic molecule is embedded in a spherically symmetric confinement. In this case, its translational degrees of freedom become quantized and can couple to electronically degenerate states in a very similar fashion as predicted by Renner-Teller effect theory. To our knowledge, it is the first time that this novel type of non-adiabatic coupling has been investigated either in theory or experiment.[1]

We demonstrate this effect for the experimentally accessible case of NO embedding in a C₆₀. Endofullerenes, in particular those carrying a radical molecule, are highly topical objects of ongoing research in molecular spectroscopy, reaction chemistry and carbon-based nanomaterial design. Also, suitable confinements in molecular traps for quantum information and quantum computing will produce a similar effect of nonadiabatic coupling as predicted by our study.

[1] A.W. Hauser and J.V. Pototschnig, *J. Phys. Chem. A*, 2022, DOI:10.1021/acs.jpca.1c10970