Hari Datt Pandey, Res. Rev. J Mat. Sci. 2018, Volume 6
DOI: 10.4172/2321-6212-C10-041

5th International Conference on
Theoretical, Materials and Condensed Matter Physics
November 26-28, 2018 | Los Angeles, USA

Estimating vibrational lifetime and boundary conductance

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Estimating vibrational signatures of a large molecular system is even tricky because of overlapping frequencies. Therefore, the vibrational probes are used to distinguish the vibrational signatures in the IR experiments. The underlying anharmonic interactions and prevailing resonances within the energy space dictate the vibrational lifetime, localization, participation, and energy flow pathway. These processes can be estimated from the quasiharmonic approximation accounting the intramolecular vibrational energy redistribution (IVR). The IVR process is irreversible and collisionless within the specified timescale of interest. We computed the IVR properties of liquid alkylbenzene systems by solving the vibrational Hamiltonian with the potential up to cubic or quartic anharmonic terms deriving the self-consistent system of nonlinear equation[1-3]. Only addressing the modes of interest and solving iteratively, the vibrational properties can be computed. Later we estimated the vibrational lifetime of the isotopically substituted nitrile probe, cyanophenylalanine[4-5]. The frequency of the nitrile of the four isotopomers decreases in the order $^{12}C^{14}N$, $^{12}C^{15}N$, $^{13}C^{14}N$, and $^{13}C^{15}N$, whereas the corresponding lifetime varies nonmonotonically with the change in frequency. The estimated lifetime first two C-N stretches are within 15% of the experimentally measured value 4.0, 2.4, 2.0, and 3.7 ps respectively and the other two are off by a factor of 2.[4-5] In the unsubstituted, $^{12}C^{14}N$, the coupled state are nonresonant at the level of cubic anharmonic interaction, whereas in other cases the energy flow is via the resonantly coupled pathway. The lifetime of $^{13}C^{15}N$ is slower contradicting the general convention that closer the resonance, faster the energy flow. We found that for some resonantly coupled modes to the CN are localized to the ring, while at other they are more delocalized. The resonantly coupled states are localized bright states and preferably is the reason behind the longer lifetime of the isotopically substituted case[4]. The IVR estimation method is also useful to determine the many-body localization-thermalization transition to estimate the boundary conductance. We have estimated the boundary conductance of various metal-alkane/perfluoroalkane-sapphier, metal-polyethylene glycol (PEG) oligomer junctions, and the results also agree with the experiments [6-11].

Biography

Hari Datt Pandey has completed his PhD in 2018 from University of Nevada Reno, USA and currently a Postdoc at University of California Riverside. He has published more than ten publications in his graduate study. His was involved in research of vibrational energy flow, and boundary conductance in the field of condensed matter physics. He was also involved in the dynamics of soft matters and currently participating in a conformational study of the protein, drug designing, and binding kinetics.

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