Role of Electron-Nuclear Coupling on Photoelectron Spectra, Reactive Scattering Processes and Phase Transition of Solids

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The first principle based Beyond Born-Oppenheimer (BBO) theory [1-3] is presented for the construction of highly accurate potentially coupled matrix (diabatic) to study multi-mode multi-surface photoelectron spectra of NO_3^- and 1,3,5-$C_6H_6F_3^+$ [4-5], reactive scattering processes of H_3^+ and $F + H_2$ [6-9], and phase transition phenomena of orthorhombic manganites [10]. Jahn-Teller (JT) and Renner-Teller (RT) types of conical intersections (CIs) along with Pseudo Jahn-Teller (PJT) interactions in those systems and semi-circular CI seam (rather than a CI point) between the ground and excited state are the new interesting observations. [4-6, 9] The theoretically calculated spectra of the titled systems show good peak by peak correspondence with the experimental and other theoretial findings. [4-5] Reaction attributes (reaction probabilities, cross-sections and/or rate constants) of $D^+ + H_2$ and $H + H_2^+$ processes obtained from scattering dynamics over global diabatic surfaces of H_3^+ system [7,8] in hyperspherical coordinates for total angular momentum zero and non-zero situations exhibit good accord with the experimentally measured ones. On the other hand, reactive scattering calculation over the diabatic surfaces of $F + H_2$ system (incorporating spin-orbit couplings) is quite encouraging. Optical spectra of $REMnO_3$ (RE = La, Pr, Nd, Sm, Eu, Gd, Tb, Dy) shows anomalous temperature dependence around the Neel temperature. This behaviour could be due to Jahn-Teller effect both in ground and excited state. Such observations have been investigated [10,11] theoretically to interpret the experimental spectra due to the excitations of the quantum rotors.

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