

Phonons, polarons and Raman scattering in layered quantum crystalline materials

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Abstract: The fundamental theory of spatially extended optical vibrational excitations, their interaction with charge carriers and the resulting polaron phenomena in multi-layer quantum crystalline materials is overviewed [1]. One of the most significant manifestations of the potential theory in multilayer planar systems and the theory of collective states in such systems is the theoretical prediction – followed by the experimental detection – of the phenomenon of propagation in superlattices of vibrational excitations of a new type, called Spatially Extended Interface Polaritons. On the grounds of the quantum theory of potential and image forces in multilayer planar systems, the dielectric function of quantum insulators is derived. Based on the quantum theory of electron emission from the ‘metal–dielectric’ structure in strong electric fields, the thermoautoelectronic emission in ‘metal–dielectric’ structures is understood as a manifestation of the quantum nature of image forces under conditions close to atomic electric fields. The behavior of the magneto-polaron resonances as a function of the phonon symmetry inherent in monolayer Transition Metal Dichalcogenides (TMDs) is unveiled [2]. Several avoided-crossing points of energy branches assisted by an optical phonon in the MP spectrum, superposition of the electron and hole states in the emerging excitations, and their impact on optical transitions in various scattering configurations are specific for these two-dimensional quantum crystalline materials [3]. The magneto-polaron resonant scattering in a monolayer TMD is explored as a function of the laser intensity and the magnetic field. The magneto-polaron resonant Raman intensity manifests three resonant splittings of double avoided-crossing levels. Three magneto-polaron excitation branches occur by virtue of the coupling of electron and hole Landau levels to an out-of-plane A_1 optical phonon mode. The energy gaps at the anticrossing points in the magneto-polaron Raman spectrum are determined for various electron and hole deformation potential constants. The derived resonant magneto-polaron Raman efficiency as a function of the magnetic field allow for exploring the relative contribution of the conduction and valence bands in TMDs to the formation of magneto-polaron excitation branches [4]. The obtained results provide a background for on-demand engineering of the optical spectra, polaron states, and transport processes in layered quantum crystalline materials towards applications in the emerging technologies encompassing artificial intelligence, quantum computing, nanotechnology, advanced materials. The support from the National Agency for Research and Development (Republic of Moldova) through the Project “ReBRAIN” no. 25.80013.5007.07RE is gratefully acknowledged.

Keywords: Phonons, Polarons, Raman scattering, Layered quantum crystalline materials, TMDs

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