Contribution ID: **26** Type: **Talk**

Electron-lattice coupling and the superconductivity in hydrogen-rich systems

Wednesday, 4 December 2019 12:45 (25 minutes)

Recent development in the high-pressure physics provides us with a new class of the superconducting materials, namely with the hydrogen-rich materials, such as silane (SiH_4, transition temperature T_c=17˜K at pressure p=96˜GPa), hydrogen sulphide ($H_{2/3}S$, T_c=203˜K @ 150˜GPa) or hydrogen lanthanide ($H_{1-x}La$, T_c=274–286˜K @ 210˜GPa).

We investigate the versatility of the molecular-to-atomic transitions in one-, two-, and quasi-three-dimensional hydrogen systems, using our own original approach – the Exact Diagonalization Ab-Initio (\textsc{edabi}) method. Starting from the extended Hubbard model, we examine an electron-correlation-driven conductivity connected with the creation of high-symmetry hydrogen molecular and atomic planes, as well as a series of both structural and electronic-in-nature quantum phase transitions.

We discuss the suppression of molecular nature in a reversed Peierls-like transition under high pressure, as well as the proper van-der-Waals-like effective interaction derived from the first principles of quantum mechanics.

Using effective electron-phonon Hamiltonian we estimate both the zero-point motion of the lattice ions, as well as the electron-lattice coupling. Next, by using the McMillan formula we estimate the superconducting transition temperature versus the effective pressure (external and/or chemical).

We acknowledge the support of National Science Centre (NCN) grant OPUS, No. UMO-2018/29/B/ST3/02646 and the European Regional Development Fund in the IT4Inno\-va\-tions national supercomputing center – path to exascale project, project number CZ 02.1.01/\-0.0\-/0.0\-/16-013/0001791 within the Operational Programme Research, Development and Education.

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