

Tight-binding Study of Compressed Solid Hydrogen

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A tight-binding(TB) approach has been used to study highly-compressed solid hydrogen. The electronic band structure calculated via TB agrees with the ab initio calculation in the valence band and resembles in conduction band. A Berry's phase approach is used to calculate the electric polarization, while we also constructed maximally-localized Wannier functions by employing the Bloch wave functions calculated from TB, then we are capable of calculating the polarization, because each wannier function can be associated with a single molecule, and the displacement of each wannier center defines a dipole momentum for the associated molecule. Both the results meet each other, and have good agreement with ab initio calculation. The spatial distribution of the wannier functions is then computed as well as the Born effective charges associated with each atom in the unit cell. The tight-binding method, therefore, provides a clear and instructive way of viewing the electronic properties in highly-compressed solid hydrogen.