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Ab initio calculation of the electron-phonon coupling for transport[1] NATHALIE VAST, JELENA SJAKSTE, PAOLA GAVA, IURII TIMROV, Laboratoire des Solides Irradiés - Ecole Polytechnique - CEA DSM - CNRS UMR7642 - France, VALERY TYUREREV, Tomsk State Pedagogical University - Russia — We have developed an approach which enables us to compute matrix elements of the electron-phonon coupling within the density functional perturbation theory for the electronic interaction with short-wavelength phonons.[2] Combining this *ab initio* approach to the Boltzmann transport equation, we have obtained the thermoelectric coefficients of silicon.[3] The lifetime of the $2p_0$ shallow impurity state in doped-silicon turns out to be shorter than expected.[4] The lifetime of the exciton in germanium under pressure[5] is found to be well described. Effect of the material nanostructuring on the electron-phonon coupling constants will be shown for small semiconducting superlattices. Finally, the calculation of deformation potentials for intravalley scattering will be discussed, and results shown for silicon and for bismuth, which is the prototype material for thermoelectricity.

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[2]J. Sjakste, N. Vast, V. Tyuterev, Phys. Rev. Lett. 99, 236405 (2007).
[3]Z. Wang, S. Wang, S. Obukhov, N. Vast, J. Sjakste, V. Tyuterev, and N. Mingo, Phys. Rev. B 83, 205208 (2011).
[4]V. Tyuterev, J. Sjakste, N. Vast, Phys. Rev. B 81, 245212 (2010)
[5]V.G. Tyuterev and S.V. Obukhov N. Vast and J. Sjakste,Phys. Rev. B 84, 035201

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