

# Semiconductor Device Theory: Bandstructure – Simulation Exercise

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Connect to the Bandstructure Lab on the nanoHUB. Choose the option for bulk bandstructure and select Si, Ge and GaAs materials. In case (1) do not select spin-orbit coupling and in case (2) select the spin-orbit coupling. Once you obtain the bulk bandstructures for the three semiconductor materials considered, answer the following questions:

- At which points in  $k$ -space is the electron effective mass smallest for the three materials considered?
- Are there points in  $k$ -space where the electron mass is negative?
- It is well established in semi-empirical band-structure calculations that the parameter set is chosen so that the experimentally measured optical gaps are fit at particular points in  $k$ -space. What are these points and how well the parameter set chosen in this theoretical model fits the experimentally measured optical gaps?
- Comment on the valence band structure behavior with and without the inclusion of spin-orbit coupling.