PREDICTION OF THERMAL RADIATIVE PROPERTIES OF SEMICONDUCTORS FROM FIRST PRINCIPLES

Hua Bao and Xiulin Ruan*
School of Mechanical Engineering and Birck Nanotechnology Center, Purdue University
585 Purdue Mall, West Lafayette, IN 47907, USA
*ruan@purdue.edu

ABSTRACT. A method based on first-principles calculations is established to predict the thermal radiative property of semiconductors from their atomic structures. In the far-infrared band, the optical absorption is due to the photon interaction with optical phonons. The dielectric function can be obtained by parameterizing the Lorentz oscillator model. In the visible band, the optical absorption of a semiconductor is due to the electron interband transitions. The dielectric function is calculated based on the GW method and Bethe–Salpeter equation. With the dielectric function, thermal radiative properties of bulk or nanomaterials can be calculated by solving the Maxwell's equations.