

Abstract Submitted
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Computing Band Structures in Undergraduate Solid State

JAVIER HASBUN, University of West Georgia — Understanding band structures is quite challenging for undergraduate solid state physics students. Calculating the band structures is even more difficult. However, using the techniques developed earlier [1], and which were applied to the simple cubic structures, it is possible to extend them to semiconducting systems in a simple way. The idea is to employ the 8-band model concept of Harrison's Hamiltonian approach [2] to model and parametrize the bands. The method also uses the system's band structure's Green's function and employs the k-space Brillouin-zone ray approach [3] combined with a complex integration method [4] to obtain the density of states. The number of occupied electron states up to a certain energy is obtained using Romberg's method and example results will be shown. [1] Javier Hasbun (J42.00013) <http://meetings.aps.org/Meeting/MAR10/Event/119248> [2] S. Froyen, and W. A. Harrison, Phys. Rev. B Vol. 20, 2420 (1979). [3] An-Ban Chen, Phys. Rev. B, Vol. 16, 3291 (1977). [4] Javier Hasbun <http://meetings.aps.org/link/BAPS.2009.MAR.L29.12>

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