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DFT Calculation of the Electronic Properties and EEL Spectrum of $NiSi_2$[1] ROBERTO NÚÑEZ-GONZÁLEZ, Departamento de Matematicas, Universidad de Sonora, ARMANDO REYES-SERRATO, DONALD H. GALVAN, Centro de Nanociencias y Nanotecnologia, UNAM, ALVARO POSADA-AMARILLAS, Departamento de Investigacion en Fisica, Universidad de Sonora — In this work we present theoretical band structure, total and projected density of states (DOS), dielectric function and electron energy-loss spectrum (EELS) of $NiSi_2$. The calculations were carried out using the Full-Potential Linearized Augmented Plane Waves (FLAPW) method, within the Density Functional Theory (DFT) with the Local Density Approximation (LDA). Our theoretical EELS results are in excellent agreement with recent experimental findings, indicating that the main peak corresponds to a plasmon. Additional peaks in our calculations are identified as interband transitions (at 2.67 eV, 4.77 eV and 6.1 eV) associated to transitions between Ni d to Si p states, and low magnitude plasmons (at 1.3 eV and 4.02 eV).

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