

Please order the Electronic structure of Na₃Bi near the Dirac point:optical measurement talk first and Electronic structure of Na₃Bi near the Dirac point:Theory talk second in the sequence.

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Electronic structure of Na₃Bi near the Dirac point: Theory¹

CHRIS LANE, B. BARBIELLINI, A. BANSIL, Northeastern U., TAY-RONG CHANG, HORNG-TAY JENG, National Tsing Hua U., H. LIN, NUS, J. KRIZAN, S. KUSHWAHA, R. CAVA, Princeton U., G. S. JENKINS, A. B. SUSHKOV, R. L. CAREY, H. D. DREW, U. of Md College Park — Band structure calculations have been performed and compared with recent optical experiments. The ground state of the system is found to be not the highly symmetric P6₃/mmc structure, but instead the P $\bar{3}$ c1 that involves buckling of the Na-Bi hexagonal planes. The band structure shows very little change between various symmetry configurations, yet the low-energy optical transition matrix elements are dramatically enhanced in the P $\bar{3}$ c1 symmetry compared with P6₃/mmc, which results in an electronic response that agrees much more closely with optical data. A peak in the joint density of states driven by the particle-hole asymmetry of the band structure along the $\Gamma - A$ momentum direction results in a large peak in the imaginary part of the dielectric function. Systematic changes are observed in the low energy Dirac cone Fermi velocity and Lifshitz gap energy with lattice spacing and spin-orbit coupling. The large anisotropies of the Dirac cone and small energy gaps are discussed.

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