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**First-Principles Study of Superconductivity in boron-doped SiC**[1]

JESSE NOFFSINGER, FELICIANO GIUSTINO, STEVEN LOUIE, MARVIN COHEN, UC Berkeley — The discovery of superconductivity in materials such as intercalated graphite, alkali-doped fullerenes, and boron-doped diamond has drawn significant interest to carbon-based superconductors. Recent experiments indicate that boron-doped cubic SiC may superconduct above 1 K [1]. We investigate the superconductivity in cubic SiC using a first-principles approach. We describe the electronic structure within density functional theory and the lattice dynamics within density functional perturbation theory. The electron-phonon interaction matrix elements are calculated via a recently developed method based on Wannier functions [2]. The boron doping is accounted for by a virtual crystal approximation. In addition to the coupling of Fermi surface electronic states to optical phonon modes, there appears to be a non-negligible contribution to the electron-phonon coupling arising from acoustic phonons. Superconductivity is discussed by analyzing the similarities and the differences with respect to the closely related boron-doped diamond. [1] Z-A. Ren et. al, *private communication*. [2] F. Giustino et. al, Phys. Rev. B 76, 165108 (2007)

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