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Theoretical and Experimental Framework of an Insulator-to-Metal Transition in Selenium-Hyperdoped Silicon ELIF ERTEKIN, University of Illinois, MARK WINKLER, Massachusetts Institute of Technology, DANIEL RECHT, AURORE SAID, MICHAEL AZIZ, Harvard University, TONIO BUONASSISI, JEFFREY GROSSMAN, Massachusetts Institute of Technology — Following the discovery of black silicon in 1998, hyperdoping - doping to concentrations orders of magnitude larger than the solubility limit - has emerged as a promising method for designing semiconductors with unique optical and electronic properties. Black silicon (silicon hyperdoped with chalcogens), synthesized by pulsed laser techniques, has recently received substantial interest owing to its broad, sub-band gap absorption down to photon energies as low as 0.5 eV, suggesting applications towards infrared detection and intermediate band photovoltaics. Until now, there has not been a clear explanation of these properties. In this presentation, we combine computational and experimental evidence to probe the origin of sub-band gap optical absorption and metallicity in black silicon. Temperature-dependent conductivity measurements show that black silicon undergoes an insulator-to-metal transition at a critical dopant concentration. Our computational analysis based on density functional theory and quantum Monte Carlo methods suggest that the enhanced optical properties result from this insulator-to-metal transition that appears to be a classic impurity-driven Mott transition, driven largely by many-body effects.

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