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Theoretical Band Offsets in c-Si/Si-XII Heterojunctions[1] JAMAL MUSTAFA, BRAD MALONE, MARVIN COHEN, STEVEN LOUIE, University of California at Berkeley and Lawrence Berkeley National Lab — Many different phases of silicon can be formed under pressure, with some being metastable at standard temperatures and pressures. For one such phase, Si-XII, experiments have recently suggested it to be a semiconductor, confirming theoretical predictions that it has a narrow gap in its electronic band structure. Current-voltage measurements show rectifying behavior in c-Si/Si-XII heterojunctions, indicative of a band discontinuity at the interface. We present computations that quantify this band discontinuity using bulk band structures obtained with Density Functional Theory within the Local Density Approximation. In particular, we demonstrate the use of a semiconductor's intrinsic charge neutrality level to determine band lineups.

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