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**DFT calculations of formation energy and properties of Frenkel pairs in Si** MATTHEW J. BECK, S. T. PANTELIDES, Department of Physics and Astronomy, Vanderbilt University, Nashville, TN — The formation of vacancy-interstitial pairs (Frenkel pairs) underlies many materials processes, including the production of defects by irradiation or ion implantation. Here we present the results of density functional calculations of the formation and properties of Frenkel pairs in Silicon for various pair configurations. The detailed relaxations and overall stability of these pairs against recombination, even at large separations, are strongly dependent on the transfer of charge among the vacancy and interstitial states in the Si band gap, and are highly sensitive to the interstitial configuration. The results are discussed with respect to their implications for models of radiation-induced defect damage and related processes. This work was supported in part by AFOSR grant FA9550-05-1-0306.

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