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Modeling of Transition Metal Color Centers in Diamond NICK GOTHARD, University of Dayton Research Institute, DOUG DUDIS, LUKE BISSELL, Air Force Research Laboratory — Diamond stands out among single-photon sources due to an intrinsically large band gap, efficient electrical excitation, the ability to host bright optical centers, photo-stable emission, room-temperature operation, short excited state lifetimes, and the ability to host hundreds of different color centers. Currently, most of these centers are active in the optical spectrum, but a single-photon source in the IR would represent a significant advancement. In pursuit of this end, the effects of a number of different transition metal atoms upon the diamond lattice have been investigated via cluster calculations using the General Atomic Molecular and Electronic Structure System (GAMESS) code. The importance of cluster size and electron correlation effects is considered, and time-dependent DFT and multi-configurational SCF approaches are compared.

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