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GPU-accelerated Search for Novel Optically Active Defects in Diamond and Silicon Carbide for Quantum Sensing Applications[1] ASHER CHOK, N. WORLEY, A. MOFFITT, H. LOVEGROVE, N. W. GOTHARD, Bob Jones University — The nitrogen-vacancy center in diamond (NV-) is the most researched color center in the field of quantum sensing. However, with hundreds of potential color centers, optically active defects may be found that demonstrate improvements in operation range or technological application as compared to the NV- site. Research into quantum sensors has explored various chemical element groups, but there is still considerable room for exploration and development. To help address this, we initiated a search for new defects in diamond and silicon carbide to determine their potential for quantum sensing application. Defect properties are calculated using density functional theory within a supercell framework with GPU-acceleration. We examined titanium, chromium, and yttrium defects in diamond, and titanium in silicon carbide. Defects are characterized with respect to formation energy, defect energy levels, and zero-phonon line (ZPL). We evaluate the sensing potential with regard to potential to form and optical accessibility.

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