

MAR17-2016-020037

Abstract for an Invited Paper
for the MAR17 Meeting of
the American Physical Society

Marshak Lectureship: Vibrational properties of isolated color centers in diamond¹

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In this talk we review our recent work on first-principles calculations of vibrational properties of isolated defect spin qubits and single photon emitters in diamond. These properties include local vibrational spectra, luminescence lineshapes, and electron-phonon coupling. They are key in understanding physical mechanisms behind spin-selective optical initialization and read-out, quantum efficiency of single-photon emitters, as well as in the experimental identification of as yet unknown centers. We first present the methodology to calculate and analyze vibrational properties of effectively isolated defect centers. We then apply the methodology to the nitrogen-vacancy and the silicon-vacancy centers in diamond. First-principles calculations yield important new insights about these important defects. Work performed in collaboration with M. W. Doherty, A. Gali, E. Londero, L. Razinkovas, and C. G. Van de Walle.

¹Supported by the Research Council of Lithuania (grant M-ERA.NET-1/2015)