## Abstract Submitted for the MAR17 Meeting of The American Physical Society

Ab-initio studies of nitrogen-vacancy impurity complexes in diamond ALEJANDRO GALLO, ANDREAS GRNEIS, Max-Planck Institute for solid state research — Nitrogen Vacancy defects in diamond have become over the last years an important candidate for a bulk room temperature quantum information processing device. We investigate the feasibility of calculating properties such as inter-system crossings between triplet and singlet levels, spin-spin interaction parameters and deformation tensors using state-of-the-art ab-initio techniques.

Alejandro Gallo Max-Planck Institute for solid state research

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