

# Electronic and optical properties and hyperfine fields of nickel-related complexes in diamond

**R. Larico<sup>1</sup>, J.F. Justo<sup>2</sup>, W.V.M. Machado<sup>3</sup> and L.V.C. Assali<sup>3</sup>**

<sup>1</sup> *Universidade Federal do ABC, Santo André, SP, Brazil*

<sup>2</sup> *Escola Politécnica, Universidade de São Paulo, São Paulo, SP, Brazil*

<sup>3</sup> *Instituto de Física Universidade de São Paulo, São Paulo, SP, Brazil*

Diamond is a material which stands alone in nature, carrying a unique combination of electronic, mechanical, thermal, and optical properties. Those properties make it a prototypical material to a number of applications, ranging from drilling and cutting tools to electronic devices used to operate under extreme conditions. More recently, new potential applications for doped diamond have been proposed, such as superconducting materials and quantum computing.

Controlled synthesis of diamond has received great attention over the last two decades. Potential applications of synthetic diamond range from mechanical tools to electronic devices. High pressure-high temperature methodology has been widely used to grow macroscopic diamond out of graphite, using transition metals alloys as solvent-catalysts.

The major problem is that the resulting material contains high concentrations of nickel extrinsic defects (dopants), forming electrically and optically active centers. It is important to understand how nickel interacts with such defects to form complexes, which may help developing processes to passivate those active centers. Therefore, there has been considerable effort to build a consistent microscopic model that could explain the experimental data on nickel-related centers [1, 2, 3, 4, 5]

Here we present a theoretical investigation, based on the spin-polarized full-potential linearized augmented plane wave (FP-LAPW) method, to investigate the atomic structures, symmetries, formation and transition energies, optical properties and hyperfine parameters of nickel-related centers in diamond. Our results of Ni impurity complex with N and B are discussed in the context of the microscopic models which have been proposed to explain the active centers in synthetic diamond [3, 4].

[1] J. Isoya et al., Phys. Rev. B 42, 9843 (1990).

[2] V.A. Nadolinny et al., J. Phys. : Condens. Matter 11, 7357 (1999).

[3] A. J. Neves et al., Diamond Relat. Mater. 9, 1057 (2000).

[4] R. N. Pereira et al., Diamond Relat. Mater. 11, 626 (2002).

[5] R. Larico, et al., Phys. Rev. B 79, 115202 (2009).