Quantum-chemical simulation of N-doped Co_3O_4

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Calculations were performed using the DFT method as implemented in the computer code VASP 5.4[1]. Core electrons were substituted with the US potentials with the PAW method [2]. Exchange-correlation described by the PBE functional [3]. The Hubbard correction *U-J*=3eV [4] was applied to *d*-electrons of Co_{tet} as well as Co_{oct} atoms [5]. For defects modeling cubic 56-atom supercell model has been used. For Brillouine zone [6] was sampled with the 2x2x2 Monkhorst-Pack scheme.

Plain-waive basis set has the kinetic energy cut-off of 550eV. Charge redistribution was analysed by the Bader method, as implemented by Henkelmann et al.

Doping by nitrogen was performed by substitution of oxygen atoms. Four concentrations have been tested – 1, 2, 4 and 8 N per 32(O+N) atoms. There are five nonequivalent distances between 32 *e* sites in the supercell – 1-4 and 6NN. Some coordination spheres are split to the subspheres with a small deviation in distances as shown in Fig. 22.

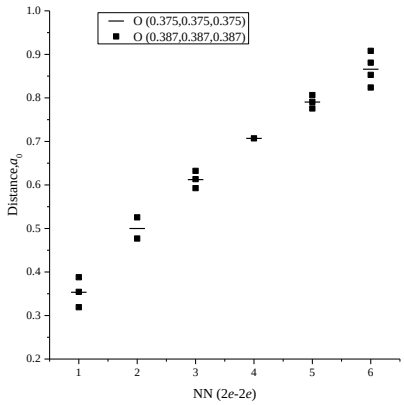

Fig. 22 Nearest Neighbours of 32*e*-32*e* sites of Co_3O_4 structure, symmetry group 227.

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[3] Perdew J.P. Phys.Rev.Lett. – 1996. – Vol. 77, – P.3865-3868.
[4] Dudarev S.L., Botton G.A., Savrasov S.Y., Humphreys C.J., Sutton A.P. Phys.Rev.B: Condens. Mater.Phys. – 1998, – Vol. 3. № 57, – P. 1505-1512.
[5] 3eV for Co (в какой-то статье говорится о том, что 3 эВ можно применять ко всем кобальтам)
[6] Monkhorst H.J., Pack J.D. Phys. Rev. B. – 1976. – Vol.13. – P. 5188-5192.