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Induction of room temperature ferromagnetism in N-doped yttrium oxide: a first-principle calculation

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Diluted magnetic semiconductors (DMS) have been gathering immense interest in spintronic devices mainly due to their unique properties of integrating photonic, electronic and magnetic on a single substrate. Traditionally, DMS are designed by doping nonmagnetic semiconductors with magnetic impurities. There are two possible ways to develop ferromagnetism (FM), such as cation/anion vacancy, and cation/anion substitution. As a result, many studies have been reported on ferromagnetic induction in nonmagnetic semiconductors by anion or cation substitution. However, there are few works on Y_2O_3. Y_2O_3 is an air-stable, solid white coloured substance. It is derived from yttrium hydroxide under heat treatment. It is used in the field of material sciences to impart colour to the television picture tubes. In this paper, we investigate the FM in N doped Y_2O_3 using the DFT calculations, and predict that a short range ferromagnetic coupling range is developed between the N impurities leading to a FM state (see Fig. 1a), which is sustainable a room temperature. The PDOS analysis and spin density plots indicate

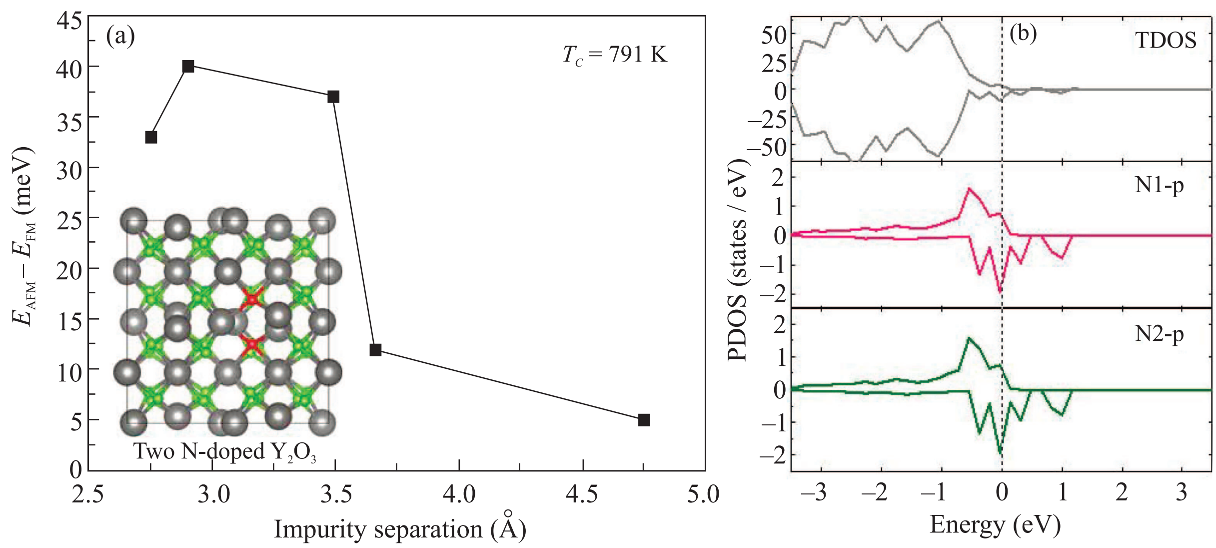

Fig. 1. (Color online) (a) – The energy difference (ΔE) between anti-ferromagnetic and ferromagnetic states corresponding to different N-N separations. (b) – Partial density of states (PDOS) for a short impurity separation (2.90 Å)

that induction of magnetic moment is possible for splitting of spin relevant to localized N-2p orbital as well as nearest Y-4d orbital, as shown in Fig. 1b. The persistence of room temperature ferromagnetism (RT-FM) has been entrenched through estimation of Curie temperature which further satisfies the demand of stability of the system. Our results show that N doped Y_2O_3 could be molded as a DMS for spintronic applications.

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