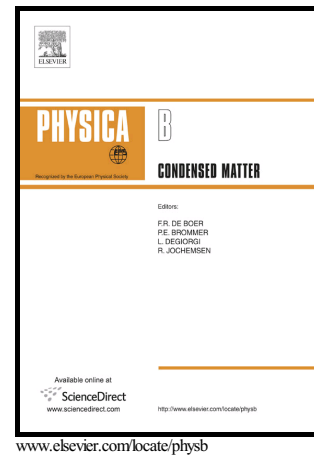


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Chemical pressure effect in magnetic frustrated pyrochlore $\text{Nd}_2\text{Pb}_2\text{O}_7$: a crystal-field analysis

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Abstract

Variation of chemical pressure at R-site due to substitution of nonmagnetic cation of varying size at the M-site makes a fine tuning between the crystal-field and molecular field to adopt exotic ground states in the frustrated magnetic $\text{R}_2\text{M}_2\text{O}_7$ pyrochlore structures. Presence of larger cation at M-site increases the lattice parameter or nearest-neighbor bond distance between magnetic R-spins, and causes subtle changes to the local oxygen environment surrounding each R-ion, thereby reduces the chemical pressure at R-sites which leads to a dramatic change in the crystal-field and molecular field at R-site. To explore the effect of chemical pressure, the experimental results of powder magnetic susceptibility and isothermal magnetization of a geometrically frustrated compound, $\text{Nd}_2\text{Pb}_2\text{O}_7$ containing largest cation, e.g. lead (Pb), at M^{4+} -sites are simulated and analyzed employing a D_{3d} crystal-field (CF) and anisotropic molecular field at R-sites in the self-consistent mean-field approach. The second-ordered axial parameter B_{20} and total CF splitting of the ground multiplet $^4I_{9/2}$ of Nd^{3+} -ions became the lowest among the isomorphic Nd-pyrochlore compounds, implying reduced effect of the crystal-field at Nd sites. $\text{Nd}_2\text{Pb}_2\text{O}_7$ has strong [111] Ising anisotropy. Relative strength and values of the exchange tensor among nearest-neighbor Nd^{3+} -spins in $\text{Nd}_2\text{Pb}_2\text{O}_7$ and $\text{Nd}_2\text{Zr}_2\text{O}_7$ results in a very close competition of anti-ferromagnetic and ferromagnetic interactions.

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