

Theoretical study of manganese melilites and related structures

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Manganese melilites and related compositions¹⁻⁸ with chemical formula of $A_2MnC'_2$ (A^{1+} : Na, K, Rb, Cs; C'^{5+} : As, V, P and A^{2+} : Ca, Sr, Ba; C'^{4+} : Si, Ge) were studied theoretically using ab initio density function theory. The relative stability of different phases was approximated by comparing relaxed crystal structure energies. Further calculations of the magnetic structure and super-super exchange parameters of selected melilite structures were also performed. The calculated results mostly agree with the limited set of experimentally measured magnetic and crystal structures^{5, 8-10} and suggest interesting pathways for further research.

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Level of Expertise

Early Career <5 Years since PdD

Do you wish to take part in the poster slam

No

Travel Funding

No

Speakers Gender

Male

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