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# Theoretical study of manganese melilites and related structures

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Manganese melilites and related compositions1-8 with chemical formula of A2MnC'2O7 (A1+: Na, K, Rb, Cs; C'5+: As, V, P and A2+: 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 structures5, 8-10 and suggest interesting pathways for further research.

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## Speakers Gender

Male

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## Level of Expertise

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No

**Primary author(s) :** SALE, Matthew (University of Sydney); XIA, Qingbo (The University of Sydney); AVDEEV, Max (Australian Nuclear Science and Technology Organisation, Australian Centre for Neutron Scattering); LING, Chris (University of Sydney)

**Presenter(s) :** SALE, Matthew (University of Sydney)

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