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【608】Non-trivial band topology in high pressure structure of $Ba_3CaIr_2O_9$

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Iridium oxides with d^5 configuration have attracted considerable interest in the last decade due to the realisation of spin-orbit-coupled (SOC) $j_{eff} = 1/2$ insulating ground states. Recently, a new class of $5d^4$ iridates with a singlet ($j_{eff} = 0$) ground states have been realised in $(Ba/Sr)_2YIrO_6$. Here, we propose a new honeycomb lattice compound $Ba_3CaIr_2O_9$ in the $j_{eff} = 0$ class of materials. Using ab initio methods including many-body wavefunction calculations we characterise the SOC ground and excited states and show that a a $j_{eff} = 0$ singlet ground state is realised. Further, we find that the material hosts non-trivial electronic band structure with a well defined Z_2 topological invariant. We analyse the effect of electronic correlations on the non-trivial bands using the Gutzwiller wavefunction approach.

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