Abstract Submitted
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First-principles design of the spinel iridate Ir_2O_4 for high temperature quantum spin ice[1] SHIGEKI ONODA, Condensed Matter Theory Laboratory, RIKEN, and Quantum Matter Theory Research Team, RIKEN Center for Emergent Matter Science, FUMIYUKI ISHII, Faculty of Mathematics and Physics, Institute of Science and Engineering, Kanazawa University — Insulating magnetic rare-earth pyrochlores related to spin ice host emergent bosonic monopolar quasiparticles. These quantum spin ice monopoles obey a magnetic analogue of quantum electrodynamics, opening a route to a magnetic analogue of electronics. However, the energy scales of the interactions among rare-earth moments are so low as 1 K that the possible quantum coherence can only be achieved at sub-Kelvins. This too low energy scale hinders advances in fundamental understandings and potential applications. Here, we desgin high-temperature quantum spin ice materials from first principles. It is shown that the *A*-site deintercalated spinel iridate Ir_2O_4, which has been experimentally grown as epitaxial thin films, is a promising candidate for quantum spin ice with a spin-ice-rule interaction of a few tens of meV. Controlling electronic structures of Ir_2O_4 through substrates, it is possible to tune magnetic interactions so that a magnetic Coulomb liquid persists at high temperatures.

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Shigeki Onoda
RIKEN, and Quantum Matter Theory Research Team

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