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## Spin wave excitations of magnetic metalorganic materials

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The Organic Materials Database (OMDB) [1,2] is an open database at Nordita that is hosting about 22,000 electronic band structures, density of states and other properties for synthesized 3-dimensional organic crystals. The web interface of the OMDB offers various search tools for the identification of novel functional materials such as band structure pattern matching and density of states similarity search. In this work we extend the OMDB to include magnetic excitation properties. For inelastic neutron scattering we focus on the dynamical structure factor  $S(Q,\omega)$  which contains information on the excitation modes of the material. We introduce a new dataset containing atomic magnetic moments and Heisenberg exchange parameters for which we calculate the spin wave spectra and dynamic structure factor with linear spin wave theory and atomistic spin dynamics [3]. We thus develop the materials informatics tools to identify topological magnon spectra such as Dirac crossings within the class of organic molecular crystals, and reveal mechanisms for the topological protection of the crossings.

### References:

- [1] S. S. Borysov, R. M. Geilhufe, and A. V. Balatsky, PloS one 12.2 (2017): e0171501.
- [2] The Organic Materials Database (OMDB), <https://omdb.mathub.io>.
- [3] J. Hellsvik, R. Díaz Pérez, R. M. Geilhufe, M. Månsson, A. V. Balatsky, in preparation.

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