in order to link the magnetic, thermal and electrical degrees of freedom, permitting theoretical models to be tested in a comprehensive manner.

Could the large thermal Hall effect in $(Zn,Fe)_2Mo_3O_8$ be useful? Enthusiasm for any prospective applications would need to be tempered by the fact that the thermal Hall effect in metals is considerably larger[6]. However, this polar magnet conducts heat relatively well for an insulator, and in principle could therefore be used as a magnetically operated heat switch. This inspires speculative ideas for applications: first in thermal logic circuits[7], where magnetic fields control the pathways taken by phonons; and second in heat pumps based on caloric materials[8], where it is necessary to control cyclical thermal processes. In heat pumps based on magnetocaloric materials, the magnetic fields required for the thermal Hall effect are necessarily already present, while in heat pumps based on electrocaloric materials, it could be attractive to have an electrically insulating heat switch in order to help prevent breakdown due to the large electrical driving fields.

Overall, multiferroic $(Zn,Fe)_2Mo_3O_8$ provides an interesting addition to the renascent field of phononics[7], as a relatively large thermal Hall effect can be dialled up using a magnetic field. In future, it will be interesting to see whether this effect can be tuned by controlling electrical polarization, or somehow exploited for applications. ❐

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MOLECULAR SEPARATION

Flexing with the flow

The tuning of metal–organic frameworks (MOFs) to control molecular adsorption has attracted considerable interest for many applications, including catalysis and molecular separation. Now, Pei-Qin Liao and colleagues report the performance of a hydrophilic MOF for the challenging separation of 1,3-butadiene (C_4H_6) from other C_4 hydrocarbons (*Science* **356,** 1193–1196; 2017).

C_4H_6 is the main ingredient for the production of synthetic rubber. It is obtained from the purification of a mixture of C_4 hydrocarbons, with impurities composing 40–70% of the total mix. However, the distillation used to remove these impurities — 1-butene (n-C_4H_8), isobutene (i-C_4H_8) and butane (C_4H_{10}), which possess similar polarizabilities, boiling points and sizes — is environmentally inefficient, requiring high temperatures and pressures that may result in polymerization of C_4H_6, impacting rubber synthesis.

MOFs separate gases via two mechanisms: thermodynamically, by binding of target (or impurity) molecules on open metal sites; or by shape selectivity of pores that permit only target (or impurity) molecules to diffuse through. Liao and colleagues screened ten different MOFs for this purpose, and measured the breakthrough curves — the amount of gas mixture that is forced through the membrane before parity is reached between concentrations of the specific compound in the inlet and outlet — for the C_4 hydrocarbons (pictured, left). Most MOFs did not permit C_4H_6 to breakthrough first, but one did, showing exceptional performance. This was Zn-BTM, where H_2btm is bis(5-methyl-1H-1,2,4-triazol-3-yl) methane. In this MOF, different breakthrough times were recorded for each C_4 hydrocarbon, enabling efficient separation. For realistic gas mixtures, the highest C_4H_6 purity was found to be 99.9%, above the 99.5% threshold required for rubber production.

The mechanism underlying this separation behaviour relies on two key factors. The first is the ability of C_4 hydrocarbons to rotate the central C–C bond, forming either a *cis* (short and thick) or a *trans* (long and thin) isomer (pictured, middle). These isomers are expected to show different adsorption energies and especially transport properties when passing through a MOF with narrow apertures. Second, the unique structure of Zn-BTM, containing a mix of discrete cavities interconnected by narrow apertures (pictured, left, inset), allows the preferential passage of C_4 hydrocarbons in the *trans* isomer (pictured, right). With respect to the other molecules, C_4H_6 has a higher barrier to adopt the *cis* configuration; in fact, X-ray diffraction experiments showed that C_4H_6 existed solely in the *trans* isomer, which most easily traverses the small apertures connecting the cavities. Using periodic density functional theory, the researchers also explored the thermodynamics of binding for all host–guest structures. They found that the other molecules have higher probability to adopt the bulkier *cis* configuration and bind to the framework more strongly than C_4H_6, both factors hindering diffusion. This combination of different bonding and diffusion selectivity for the *trans* isomer of C_4H_6 resulted in substantially faster transport through the MOF, and a more efficient separation from the other C_4 molecules.

It would be interesting to see if this approach of manipulating molecule isomer structure could be utilized for larger and more complicated molecules, but, as it is, this work demonstrates the potential for MOFs with well-controlled cavity networks to be used for advanced gas separation applications.

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