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Computational materials: Open data settled in materials theory

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Your concerns over impediments to data sharing (*Nature* **546**, 327; 2017) are no longer an issue in computational materials science. This is because the Novel Materials Discovery project (NOMAD; https://nomad-coe.eu) has stimulated a cultural shift in attitudes towards open data as a result of the valuable knowledge that has emerged from data mining since early 2014.

NOMAD provides open access to input and output files from the field's major data collections (including http://aflowlib.org; http://oqmd.org; and https://materialsproject.org), together with those of individual researchers and groups. It contains more than 40 million total-energy calculations, corresponding to billions of core processing hours by high-performance computers globally.

NOMAD hosts the data for a decade or more, offers digital object identifiers (DOIs) to make data citable, and provides services such as an encyclopaedia, big-data analytics tools and advanced graphics.

Hosting the data is expensive, so funding agencies need to step in. However, costs are negligible compared with those of data creation and long-term storage.

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