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Functional materials discovery using energy–structure–function maps

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Computational data related to landscapes of predicted crystal structures (see Table D1), energy-structure-function (ESF) maps (see Table D2-D3) and predicted thermal stability of predicted crystal structures (see Table D4) have been deposited in a series of files that can be accessed via DOI http://doi.org/10.5258/SOTON/404749. Further description of the deposited data can be found within the individual files.

Table D1. Predicted crystal structures of molecules **T0, T1, T2, T2E, S1, S2, P1, P2, P1M** and **P2M** with relative lattice energies (E_{rel}) within 100 kJ mol^{-1} from the corresponding global minimum.

File name	File content description
T0_Predicted_Structures.cif	**T0** predicted crystal structures with E_{rel} below 100 kJ mol^{-1}.
T1_Predicted_Structures.cif	**T1** predicted crystal structures with E_{rel} below 100 kJ mol^{-1}.
T2_Predicted_Structures.cif	**T2** predicted crystal structures with E_{rel} below 100 kJ mol^{-1}.
T2E_Predicted_Structures.cif	**T2E** predicted crystal structures with E_{rel} below 100 kJ mol^{-1}.
S1_Predicted_Structures.cif	**S1** predicted crystal structures with E_{rel} below 100 kJ mol^{-1}.
S2_Predicted_Structures.cif	**S2** predicted crystal structures with E_{rel} below 100 kJ mol^{-1}.
P1_Predicted_Structures.cif	**P1** predicted crystal structures with E_{rel} below 100 kJ mol^{-1}.
P2_Predicted_Structures.cif	**P2** predicted crystal structures with E_{rel} below 100 kJ mol^{-1}.
P1M_Predicted_Structures.cif	**P1M** predicted crystal structures with E_{rel} below 100 kJ mol^{-1}.
P2M_Predicted_Structures.cif	**P2M** predicted crystal structures with E_{rel} below 100 kJ mol^{-1}.

Table D2. ESF maps. Calculated properties of predicted crystal structures, with relative lattice energies within 100 kJ mol^{-1} from the corresponding global minimum, of **T0, T1, T2, T2E, S1, S2, P1, P2, P1M** and **P2M** molecules.

File name	File content description
T0_ESF_maps.txt	Pore dimensionality (PD), maximum free sphere (D_f), isosteric heat (Q_{st}), methane volumetric capacity at 5.8 bar ($MVU_{5.8}$), methane volumetric capacity at 65 bar (MVU_{65}) and methane deliverable capacity (MDC) of **T0** predicted crystal structures.
T1_ESF_maps.txt	PD, D_f, Q_{st}, $MVU_{5.8}$, MVU_{65} and MDC of **T1** predicted crystal structures.
T2_ESF_maps.txt	PD, D_f, Q_{st}, $MVU_{5.8}$, MVU_{65} and MDC of **T2** predicted crystal structures.
T2E_ESF_maps.txt	PD, D_f, Q_{st}, $MVU_{5.8}$, MVU_{65} and MDC of **T2E** predicted crystal structures.
S1_ESF_maps.txt	PD, D_f, Q_{st}, $MVU_{5.8}$, MVU_{65} and MDC of **S1** predicted crystal structures.
S2_ESF_maps.txt	PD, D_f, Q_{st}, $MVU_{5.8}$, MVU_{65} and MDC of **S2** predicted crystal structures.
P1_ESF_maps.txt	PD and D_f of **P1** predicted crystal structures.
P2_ESF_maps.txt	PD, D_f, Q_{st}, $MVU_{5.8}$, MVU_{65} and MDC of **P2** predicted crystal structures.
P1M_ESF_maps.txt	PD, D_f, Q_{st}, $MVU_{5.8}$, MVU_{65} and MDC of **P1M** predicted crystal structures.
P2M_ESF_maps.txt	PD, D_f, Q_{st}, $MVU_{5.8}$, MVU_{65} and MDC of **P2M** predicted crystal structures.

Table D3. Hydrogen deliverable capacity and hydrocarbon separation results of selected **T2** leading edge predicted structures.

File name	File content description
T2_H2_Deliverable_Capacity.txt	H_2 deliverable capacity of selected **T2** leading edge predicted crystal structures.
T2_Propane_Methane_Separeation.txt	Propane/Methane separation results for selected **T2** leading edge predicted crystal structures.
T2_Propane_Propene_Separeation.txt	Propane/Propene separation results for selected **T2** leading edge predicted crystal structures.
T2_Xylene_Isomers_Separeation.txt	Xylene (*orto*-, *meta*- and *para*-) separation results for selected **T2** leading edge predicted crystal structures.

Table D4. Thermal stability of selected **T0**, **T1** and **T2** leading edge predicted structures at 300 K.

File name	File content description
T0_Thermal_Stability_Results.txt	Thermal stability results for selected **T0** leading edge predicted crystal structures.
T1_Thermal_Stability_Results.txt	Thermal stability results for selected **T1** leading edge predicted crystal structures.
T2_Thermal_Stability_Results.txt	Thermal stability results for selected **T2** leading edge predicted crystal structures.