

Supporting Information

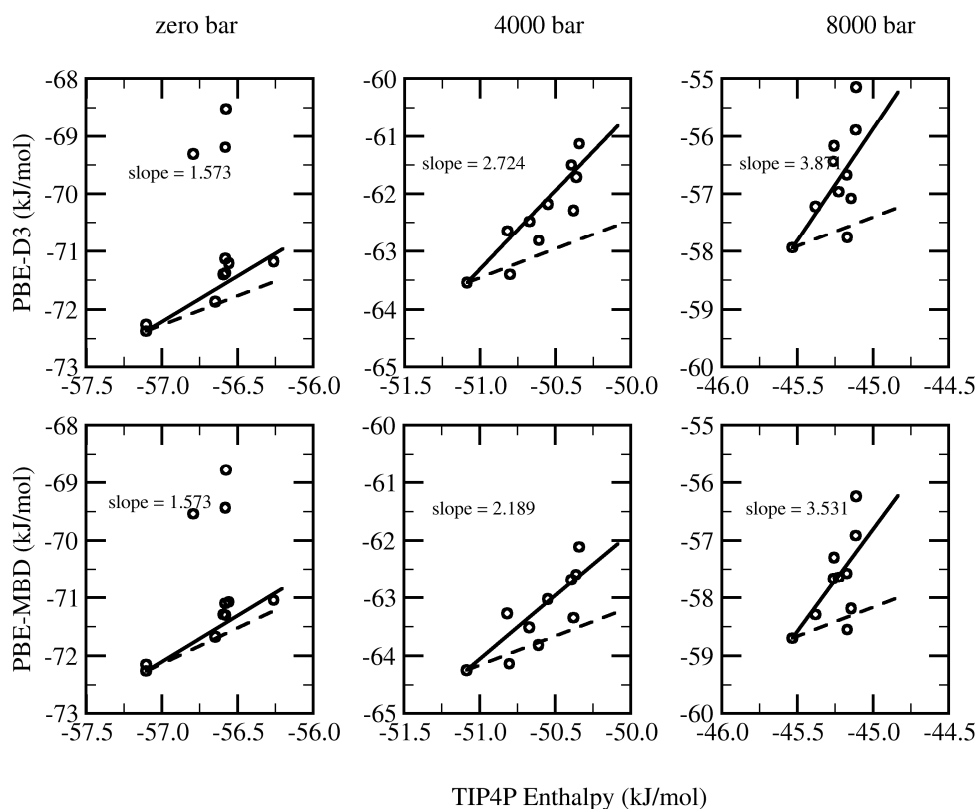
# Stability-Ranking of Crystalline Ice Polymorphs using Density-Functional Theory

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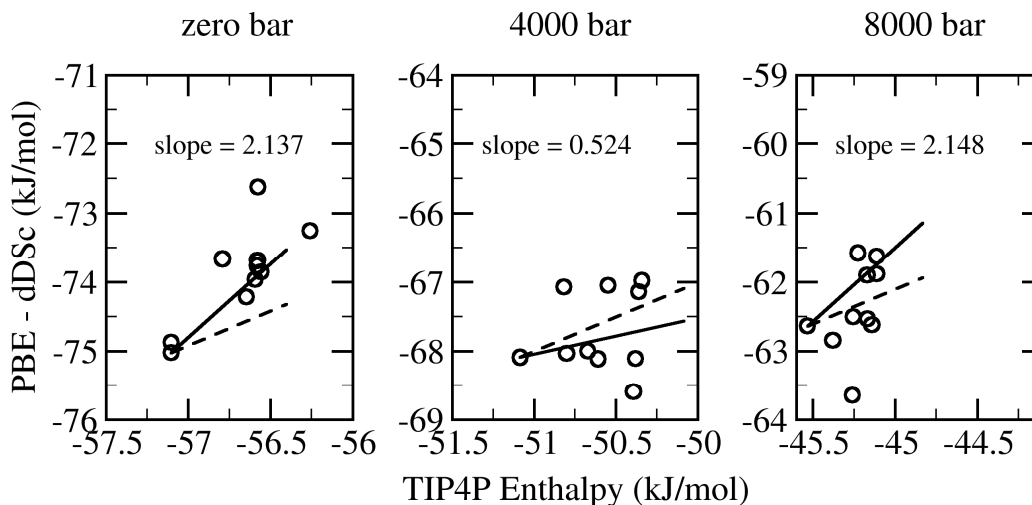
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**Figure S1.** Density-Functional Theory (DFT) (PBE-D3 and PBE-MBD)-predicted energy against TIP4P energy. The slopes of DFT (PBE-D3 and PBE-MBD) energy with respect to TIP4P energy at 0 bar, 4000 bar and 8000 bar of external pressure, respectively. Dash (---) is the line with slope of unity.



**Figure S2.** DFT (PBE-D3 and PBE-MBD) predicted energy against TIP4P energy considering the density-dependent dispersion correction (dDsC) dispersion interaction. The slopes of DFT energy with respect to TIP4P energy at 0 bar, 4000 bar and 8000 bar of external pressure, respectively. Dash (---) is the line with slope of unity.

**Table S1.** Comparison between TIP4P- and DFT-Predicted Ten Lowest-Enthalpy-per-Molecule Structures at 0 bar.

Structure	TIP4P	PBE-D3	PBE-MBD	PBE-dDsC
S4/6 <sup>8</sup> (ice Ic)	-57.104	-72.261	-72.592	-75.023
S8/6 <sup>16</sup> (ice Ih)	-57.104	-72.374	-72.721	-74.871
S12/5 <sup>8</sup> 7 <sup>8</sup> 8 <sup>8</sup> (ice III)	-56.793	-69.310	-69.943	-73.659
S12/4 <sup>1</sup> 6 <sup>20</sup> 8 <sup>10</sup>	-56.647	-71.866	-72.196	-74.215
S14/5 <sup>2</sup> 6 <sup>22</sup> 7 <sup>2</sup> 8 <sup>6</sup>	-56.593	-71.399	-71.754	-73.659
S14/6 <sup>28</sup> 8 <sup>4</sup>	-56.581	-71.126	-71.496	-73.760
S12/5 <sup>8</sup> 6 <sup>2</sup> 7 <sup>4</sup> 8 <sup>6</sup>	-56.580	-69.196	-69.865	-73.679
S12/5 <sup>8</sup> 6 <sup>4</sup> 7 <sup>8</sup> 8 <sup>8</sup>	-56.578	-71.376	-71.710	-73.689
S12/4 <sup>2</sup> 5 <sup>4</sup> 6 <sup>4</sup> 7 <sup>8</sup> 8 <sup>6</sup>	-56.577	-68.523	-69.081	-72.626
S12/5 <sup>2</sup> 6 <sup>16</sup> 7 <sup>8</sup>	-56.557	-71.208	-71.594	-73.853
...	...	...	...	...
S6/5 <sup>6</sup> 8 <sup>6</sup>	-56.260	-71.178	-71.526	-73.252

\*TIP4P energies are taken from Ref. (14).

**Table S2.** Comparison between TIP4P- and DFT-Predicted Ten Lowest-Enthalpy-per-Molecule Structures at 4000 bar.

Structure	TIP4P	PBE-D3	PBE-MBD	PBE-dDsC
S12/5 <sup>8</sup> 7 <sup>8</sup> 8 <sup>8</sup> (ice III)	-51.086	-63.540	-64.246	-68.089
S12/4 <sup>2</sup> 5 <sup>4</sup> 6 <sup>4</sup> 7 <sup>8</sup> 8 <sup>6</sup>	-50.818	-62.649	-63.272	-67.073
S12/5 <sup>8</sup> 6 <sup>2</sup> 7 <sup>4</sup> 8 <sup>6</sup>	-50.802	-63.401	-64.138	-68.036

Structure	TIP4P	PBE-D3	PBE-MBD	PBE-dDsC
S12/4 <sup>2</sup> 6 <sup>8</sup> 8 <sup>22</sup> 10 <sup>30</sup>	-50.672	-62.484	-63.513	-68.000
S12/6 <sup>14</sup> 8 <sup>18</sup> 10 <sup>30</sup> (ice II)	-50.609	-62.815	-63.815	-68.112
S12/5 <sup>6</sup> 6 <sup>6</sup> 7 <sup>4</sup> 8 <sup>8</sup> 9 <sup>4</sup>	-50.548	-62.179	-63.025	-67.049
S6/7 <sup>8</sup> 8 <sup>12</sup>	-50.394	-61.503	-62.685	-68.591
S14/4 <sup>4</sup> 5 <sup>6</sup> 6 <sup>4</sup> 8 <sup>6</sup> 9 <sup>4</sup> 10 <sup>24</sup>	-50.380	-62.290	-63.348	-68.107
S14/5 <sup>7</sup> 6 <sup>17</sup> 8 <sup>10</sup> 9 <sup>6</sup> 10 <sup>1</sup>	-50.362	-61.710	-62.597	-68.142
S10/5 <sup>4</sup> 6 <sup>2</sup> 7 <sup>4</sup> 8 <sup>16</sup>	-50.342	-61.134	-62.115	-66.976
...	...	...	...	...
S10/4 <sup>10</sup> 8 <sup>18</sup> (ice VI)	-49.989	-60.780	-62.025	-67.287

**Table S3.** Comparison between TIP4P- and DFT-Predicted Ten Lowest-Enthalpy-per-Molecule Structures at 8000 bar.

Structure	TIP4P	PBE-D3	PBE-MBD	PBE-dDsC
S12/5 <sup>8</sup> 7 <sup>8</sup> 8 <sup>8</sup> (ice III)	-45.533	-57.940	-58.699	-62.638
S12/4 <sup>2</sup> 6 <sup>8</sup> 8 <sup>22</sup> 10 <sup>30</sup>	-45.380	-57.223	-58.294	-62.844
S6/7 <sup>8</sup> 8 <sup>12</sup> (ice XII)	-45.261	-56.443	-57.669	-63.643
S14/6 <sup>10</sup> 7 <sup>16</sup> 8 <sup>20</sup> 9 <sup>8</sup>	-45.256	-56.167	-57.299	-62.595
S12/4 <sup>2</sup> 5 <sup>4</sup> 6 <sup>4</sup> 7 <sup>8</sup> 8 <sup>6</sup>	-45.227	-56.967	-57.646	-61.573
S12/5 <sup>6</sup> 6 <sup>6</sup> 7 <sup>4</sup> 8 <sup>8</sup> 9 <sup>4</sup>	-45.172	-56.677	-57.578	-61.899
S12/5 <sup>8</sup> 6 <sup>2</sup> 7 <sup>4</sup> 8 <sup>6</sup>	-45.169	-57.758	-58.552	-62.532
S14/4 <sup>4</sup> 5 <sup>6</sup> 6 <sup>4</sup> 8 <sup>6</sup> 9 <sup>4</sup> 10 <sup>24</sup>	-45.143	-57.083	-58.184	-62.618
S10/5 <sup>4</sup> 6 <sup>2</sup> 7 <sup>4</sup> 8 <sup>16</sup>	-45.114	-55.894	-56.919	-61.879
S8/4 <sup>2</sup> 7 <sup>4</sup> 8 <sup>20</sup> 9 <sup>4</sup>	-45.112	-55.146	-56.237	-61.622
...	...	...	...	...
S2/6 <sup>4</sup> (ice VII)	-39.691	-50.133	-51.536	-60.787

**Table S4.** Comparison between TIP4P- and DFT-Predicted Densities at 0 bar.

Structure	TIP4P	PBE-D3	PBE-MBD	PBE-dDsC
S4/6 <sup>8</sup> (ice Ic)	0.977023	1.030991	1.036394	1.058680
S8/6 <sup>16</sup> (ice Ih)	0.978662	1.032281	1.036394	1.056949
S12/5 <sup>8</sup> 7 <sup>8</sup> 8 <sup>8</sup> (ice III)	1.242597	1.243372	1.251217	1.312961
S12/4 <sup>1</sup> 6 <sup>20</sup> 8 <sup>10</sup>	0.959639	1.013881	1.018109	1.038283
S14/5 <sup>2</sup> 6 <sup>22</sup> 7 <sup>2</sup> 8 <sup>6</sup>	0.977531	1.029667	1.034858	1.056929
S14/6 <sup>2</sup> 8 <sup>4</sup>	0.998033	1.047124	1.052255	1.074724
S12/5 <sup>8</sup> 6 <sup>2</sup> 7 <sup>4</sup> 8 <sup>6</sup>	1.228561	1.239037	1.246524	1.303236
S12/5 <sup>8</sup> 6 <sup>4</sup> 7 <sup>8</sup> 8 <sup>8</sup>	0.947229	0.997372	1.002078	1.020947

Structure	TIP4P	PBE-D3	PBE-MBD	PBE-dDsC
S12/4 <sup>2</sup> 5 <sup>4</sup> 6 <sup>4</sup> 7 <sup>8</sup> 8 <sup>6</sup>	1.228183	1.222285	1.225415	1.308366
S12/5 <sup>2</sup> 6 <sup>16</sup> 7 <sup>8</sup>	0.985920	1.040963	1.046396	1.068386
...	...	...	...	...
S6/5 <sup>6</sup> 8 <sup>6</sup>	0.894626	0.946979	0.95039	0.968495

\*TIP4P energies are taken from Ref. (14).

**Table S5.** Comparison between TIP4P- and DFT-Predicted Densities at 4000 bar.

Structure	TIP4P	PBE-D3	PBE-MBD	PBE-dDsC
S12/5 <sup>8</sup> 7 <sup>8</sup> 8 <sup>8</sup> (ice III)	1.281094	1.280226	1.286789	1.346454
S12/4 <sup>2</sup> 5 <sup>4</sup> 6 <sup>4</sup> 7 <sup>8</sup> 8 <sup>6</sup>	1.271653	1.264263	1.267298	1.333547
S12/5 <sup>8</sup> 6 <sup>2</sup> 7 <sup>4</sup> 8 <sup>6</sup>	1.349745	1.366497	1.278857	1.332903
S12/4 <sup>2</sup> 6 <sup>8</sup> 8 <sup>22</sup> 10 <sup>30</sup>	1.288406	1.318362	1.371457	1.433804
S12/6 <sup>14</sup> 8 <sup>18</sup> 10 <sup>30</sup> (ice II)	1.288406	1.318362	1.322637	1.379522
S12/5 <sup>6</sup> 6 <sup>6</sup> 7 <sup>4</sup> 8 <sup>8</sup> 9 <sup>4</sup>	1.321323	1.308796	1.315801	1.397462
S6/7 <sup>8</sup> 8 <sup>12</sup>	1.392906	1.419570	1.424528	1.472086
S14/4 <sup>4</sup> 5 <sup>6</sup> 6 <sup>4</sup> 8 <sup>6</sup> 9 <sup>4</sup> 10 <sup>24</sup>	1.363723	1.382133	1.388227	1.453622
S14/5 <sup>7</sup> 6 <sup>17</sup> 9 <sup>8</sup> 10 <sup>9</sup> 6 <sup>10</sup> 1	1.331462	1.350790	1.356390	1.417936
S10/5 <sup>4</sup> 6 <sup>2</sup> 7 <sup>4</sup> 8 <sup>16</sup>	1.366768	1.371782	1.377341	1.442714
...	...	...	...	...
S10/4 <sup>10</sup> 8 <sup>18</sup> (ice VI)	1.443410	1.460823	1.464829	1.542645

**Table S6.** Comparison between TIP4P- and DFT-Predicted Densities at 8000 bar.

Structure	TIP4P	PBE-D3	PBE-MBD	PBE-dDsC
S12/5 <sup>8</sup> 7 <sup>8</sup> 8 <sup>8</sup> (ice III)	1.311953	1.311713	1.331568	1.374030
S12/4 <sup>2</sup> 6 <sup>8</sup> 8 <sup>22</sup> 10 <sup>30</sup>	1.372716	1.385754	1.393880	1.454665
S6/7 <sup>8</sup> 8 <sup>12</sup> (ice XII)	1.414089	1.439266	1.449613	1.494645
S14/6 <sup>10</sup> 7 <sup>16</sup> 8 <sup>20</sup> 9 <sup>8</sup>	1.433910	1.441264	1.451304	1.527318
S12/4 <sup>2</sup> 5 <sup>4</sup> 6 <sup>4</sup> 7 <sup>8</sup> 8 <sup>6</sup>	1.304657	1.305511	1.314740	1.364056
S12/5 <sup>6</sup> 6 <sup>6</sup> 7 <sup>4</sup> 8 <sup>8</sup> 9 <sup>4</sup>	1.358172	1.356581	1.356940	1.418280
S12/5 <sup>8</sup> 6 <sup>2</sup> 7 <sup>4</sup> 8 <sup>6</sup>	1.293327	1.301110	1.307747	1.360386
S14/4 <sup>4</sup> 5 <sup>6</sup> 6 <sup>4</sup> 8 <sup>6</sup> 9 <sup>4</sup> 10 <sup>24</sup>	1.387905	1.414870	1.415779	1.479716
S10/5 <sup>4</sup> 6 <sup>2</sup> 7 <sup>4</sup> 8 <sup>16</sup>	1.389176	1.388144	1.385893	1.470229
S8/4 <sup>2</sup> 7 <sup>4</sup> 8 <sup>20</sup> 9 <sup>4</sup>	1.428980	1.432488	1.436788	1.512533
...	...	...	...	...
S2/6 <sup>4</sup> (ice VII)	1.605063	1.635786	1.629991	1.791039