Supplementary Material for

Periodic Density Functional Theory (PDFT) Simulating Crystal Structures with Microporous CHA Framework: an Accuracy and Efficiency Study

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Table S1 Geometric parameters of zeolite chabazite HSSZ-13 (T = Si) reported in the neutron scattering experiment.

parameter	value	parameter	value
T-O(1)	1.617 Å	∠T-O(2)-Si(2)	149.42°
T-O(2)	1.600 Å	∠T-O(3)-Si(3)	147.79°
T-O(3)	1.615 Å	∠T-O(4)-Si(4)	149.94°
T-O(4)	1.613 Å	∠O(1)-T-O(2)	110.33°
Si(1)-O(1)	1.617 Å	∠O(1)-T-O(3)	110.21°
Si(2)-O(2)	1.600 Å	∠O(1)-T-O(4)	107.88°
Si(3)-O(3)	1.615 Å	∠O(2)-T-O(3)	109.71°
Si(4)-O(4)	1.613 Å	∠O(2)-T-O(4)	108.42°
∠T-O(1)- Si(1)	144.73°	∠O(3)-T-O(4)	110.26°

Table S2 Geometrical parameters of Zeolite HSAPO34 (T = P) reported in the neutron scattering experiment.

parameter	value	parameter	value
T-O(1)	1.502 Å	∠T-O(2)-Al (2)	149.26°
T-O(2)	1.550 Å	∠T-O(3)-Al (3)	150.36°
T-O(3)	1.589 Å	∠T-O(4)-Al (4)	150.55°
T-O(4)	1.589 Å	∠O(1)-T-O(2)	110.81°
Al(1)-O(1)	1.815 Å	∠O(1)-T-O(3)	110.69°
Al(2)-O(2)	1.682 Å	∠O(1)-T-O(4)	107.37°
Al(3)-O(3)	1.682 Å	∠O(2)-T-O(3)	112.02°
Al(4)-O(4)	1.652 Å	∠O(2)-T-O(4)	107.39°
∠T-O(1)- Al(1)	143.63°	∠O(3)-T-O(4)	108.37°

Table S3 The structure of all-silica chabazite optimized by PBE_mGGA.

element	x	y	z
Si	0.10555	0.33233	0.87827
Si	0.89445	0.66767	0.12173
Si	0.87828	0.10556	0.33233
Si	0.12173	0.89444	0.66766
Si	0.33233	0.87827	0.10556
Si	0.66767	0.12173	0.89444
Si	0.66767	0.89445	0.12173
Si	0.33233	0.10555	0.87827
Si	0.89445	0.12173	0.66766
Si	0.10555	0.87828	0.33233
Si	0.12173	0.66767	0.89444
Si	0.87827	0.33233	0.10556
O	0.02651	0.31693	0.02651
O	0.97349	0.68307	0.97349
O	0.02651	0.02651	0.31693
O	0.97349	0.97349	0.68307
O	0.31693	0.02651	0.02651
O	0.68307	0.97349	0.97349
O	0.14581	0.50000	0.85419
O	0.85419	0.50000	0.14581
O	0.85419	0.14581	0.50000
O	0.14581	0.85419	0.50000
O	0.50000	0.85419	0.14581
O	0.50000	0.14581	0.85419
O	0.25418	0.25418	0.89228
O	0.74582	0.74582	0.10772
O	0.89228	0.25418	0.25418
O	0.10772	0.74582	0.74583
O	0.25418	0.89228	0.25417
O	0.74582	0.10772	0.74582
O	1.00000	0.26031	0.73969
O	-0.00000	0.73968	0.26031
O	0.73968	-0.00000	0.26031
O	0.26032	1.00000	0.73969
O	0.26031	0.73969	-0.00000
O	0.73969	0.26031	-0.00000

Table S4 The structure of AlPO$_4$-34 framework optimized by PBE_mGGA.

index	element	x	y	z
1	P	0.11080	0.33269	0.87871
2	P	0.88920	0.66731	0.12129
3	P	0.87871	0.11079	0.33269
4	P	0.12129	0.88921	0.66731
5	P	0.33269	0.87871	0.11080
6	P	0.66731	0.12129	0.88920
7	Al	0.66789	0.89999	0.12289
8	Al	0.33211	0.10001	0.87711
9	Al	0.90000	0.12289	0.66789
10	Al	0.10000	0.87711	0.33211
11	Al	0.12289	0.66789	0.90000
12	Al	0.87711	0.33211	0.10000
13	O	0.03486	0.31710	0.01623
14	O	0.96514	0.68290	0.98377
15	O	0.01623	0.03486	0.31710
16	O	0.98377	0.96514	0.68290
17	O	0.31710	0.01623	0.03486
18	O	0.68290	0.98377	0.96514
19	O	0.15057	0.49004	0.85926
20	O	0.84943	0.50996	0.14074
21	O	0.85926	0.15057	0.49004
22	O	0.14074	0.84943	0.50996
23	O	0.49004	0.85926	0.15057
24	O	0.50996	0.14074	0.84943
25	O	0.24889	0.25776	0.89175
26	O	0.75111	0.74224	0.10825
27	O	0.89175	0.24889	0.25776
28	O	0.10825	0.75111	0.74224
29	O	0.25776	0.89175	0.24889
30	O	0.74224	0.10825	0.75111
31	O	0.01292	0.26799	0.74738
32	O	0.98708	0.73201	0.25262
33	O	0.74738	0.01292	0.26799
34	O	0.25262	0.98708	0.73201
35	O	0.26799	0.74738	0.01291
36	O	0.73201	0.25262	0.98709

Table S5 The information on seven sets of pseudopotentials selected in this study.

index	pseudopotential category	"TITEL" in POTCAR				"LEXCH" in POTCAR
		Si	Al	P	O	Si, Al, P, and O
a)	USPP_LDA	US Si	US Al	US P	US O	CA
b)	USPP_GGA	US Si	US Al	US P	US O	91
c)	LDA_PP	PAW Si 02Apr 1999	PAW Al 17Apr2000	PAW P 26Mar2009	PAW O 22Mar2012	91
d)	PAW_GGA	PAW_GGA Si 05Jan2001	PAW_GGA Al 5Jan2001	PAW_GGA P 21Jan2003	PAW_GGA O 05Jan2001	91
e)	PAW_PBE	PAW_PBE Si 05Jan2001	PAW_PBE Al 4Jan2001	PAW_PBE P 17Jan2003	PAW_PBE O 8Apr2002	PE
f)	PBE_GW	PAW_PBE Si_GW 04May2012	PAW_PBE Al_GW 19Mar2012	PAW_PBE P_GW 19Mar2012	PAW_PBE O_GW 19Mar2012	PE
g)	PBE_mGGA	PAW_PBE Si 05Jan2001	PAW_PBE Al 4Jan2001	PAW_PBE P 17Jan2003	PAW_PBE O 8Apr2002	PE

Notes:

1) The meanings of variables of "TITLE = …" are following:

"TITLE = US Si" refers to the ultrasoft pseudopotential for Si atom.

"TITLE = US P" refers to the ultrasoft pseudopotential for P atom.

"TITLE = PAW Si 02Apr 1999" refers to the projector augmented wave (PAW) potential for Si atom, which built up at about 02 Apr, 1999.

"TITLE = PAW_GGA Si 05Jan2001" refers to the projector augmented wave (PAW) potential with general gradient approximation for Si atom, which built up at about 02 Apr, 1999.

"TITLE = PAW_PBE Si 05Jan2001" refers to the projector augmented wave (PAW) potential with the implemented Perdew-Burke-Ernzerh of functional (PAW_PBE) for Si atom, which is built up at about 05Jan2001.

"TITLE = PAW_PBE Si_GW 04May2012" refers to the GW potentials with the implemented Perdew-Burke-Ernzerh (PBE_GW) for Si atom, which is built up at 04May2012.

PBE_mGGA refers to strongly constrained and appropriately normed (SCAN) meta-generalized-gradient approximation (meta-GGA) with the implemented Perdew-Burke-Ernzerh of functional (PBE-mGGA).

2) The meanings of variables of "LEXCH" are following:

"LEXCH = CA" means that the exchange-correlation energy functional is the format of local density approximation of Ceperly and Alder (CA) parameterized by J. Perdew and Zunger.

LEXCH = GGA" means that the exchange-correlation energy functional is the format of general gradient approximation (GGA);

LEXCH = 91" means that the exchange-correlation energy functional is the format of Perdew Wang 91 (91) approximation;

LEXCH = PE" means that the exchange-correlation energy functional is the format of Perdew-Burke Ernzerhof (PE) approximation.