Supporting Information

Fast screening of porous material for noble gas adsorption and separation: a classical density functional approach

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Table S1 The mapping from code E-*n* to the name of the adsorbents in Chung *et al*.'s database

In file "Table_S1.xlsx"

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Table S2 The most favorable separation adsorbents and their separation efficiencies (S_E), selectivity and uptakes.

Class	*i/j*	Adsorbent	$S_E(i/j)$	S_{ij}	Uptake mol/L
1	Ne/He	E-564	5.8	5.6	0.14
2	Ar/He	E-164	16067.7	502.4	3.77
3	Kr/He	H-371	1175.2	267.8	8.73
4	Xe/He	H-330	1137.9	239.7	8.63
5	Rn/He	E-42	2245.1	410.6	15.48
6	Ar/Ne	E-255	457.2	45.2	4.97
7	Kr/Ne	H-371	914.5	38.0	8.73
8	Xe/Ne	H-330	1010.9	128.6	8.64
9	Rn/Ne	E-42	2174.3	339.6	15.48
10	Kr/Ar	E-2027	399.8	20.9	5.45
11	Xe/Ar	H-330	574.9	15.8	8.63
12	Rn/Ar	E-42	1897.2	161.6	15.48
13	Xe/Kr	E-204	312.8	8.7	5.99
14	Rn/Kr	E-1421	1897.2	103.2	8.77
15	Rn/Xe	E-42	1420.5	45.0	15.48
16	He/Ne	E-794	0.02	2.12	1.1×10^{-3}
17	He/Ar	E-2111	0.9	1.3×10^{4}	3.9×10^{-3}
18	He/Kr	E-333	2.5	8.2×10^{6}	6.6×10^{-3}
19	He/Xe	E-333	8.1	1.6×10^{22}	6.6×10^{-3}
20	He/Rn	E-333	11.2	3.4×10^{30}	6.6×10^{-3}
21	Ne/Ar	E-333	1.4	229.7	0.01
22	Ne/Kr	E-2589	4.4	6.6×10^{5}	0.01
23	Ne/Xe	E-3474	18.1	4.7×10^{12}	0.03
24	Ne/Rn	E-3474	25.0	3.7×10^{17}	0.03
25	Ar/Kr	E-1426	10.8	9.0	0.20
26	Ar/Xe	E-1440	869.2	1.0×10^{4}	3.90
27	Ar/Kr	E-1440	1168.3	2.5×10^{5}	3.90
28	Kr/Xe	E-1440	903.9	1.1×10^{4}	4.04
29	Kr/Rn	E-1440	1213.8	2.5×10^{5}	4.04
30	Xe/Rn	E-1564	449.8	56.8	4.62

Numerical algorithm

In CDFT, the most time consuming procedure is the 3-dimensional convolution integral such as equation (11), (14) and (19) in the main text. By using ordinary integration method, this implies a 6-loop in the code, which makes the program extremely inefficient (approximately 150 CPU hours per each system). In this work, the Fast Fourier transform was used to deal with this problem, which transform the convolution integral into:

$$\int f_1(\boldsymbol{r}) f_2(\boldsymbol{r}-\boldsymbol{r}')\mathrm{d}\boldsymbol{r}' = \mathcal{F}^{-1}\{\mathcal{F}[f_1(\boldsymbol{r})]\mathcal{F}[f_2(\boldsymbol{r})]\} \quad \backslash^* \text{ MERGEFORMAT (S1)}$$

where $\mathcal{F}$ and $\mathcal{F}^{-1}$ are the forward and the backward fast Fourier transform, which was implemented by the FFTW3 package.[1] By using this treatment, the computational efficiency was improved by 10^5 times from the ordinary numerical integration.

Other integrations were coded by using discrete integration method:

$$\int f(\boldsymbol{r})\mathrm{d}\boldsymbol{r} = \sum_{\mathbf{r}} f(\boldsymbol{r})\Delta x\Delta y\Delta z \quad \backslash^* \text{ MERGEFORMAT (S2)}$$

The external potential $V_{\mathrm{ext}}(\mathbf{r})$ was pre-tabulated before the CDFT calculation by using equation (1) and (5) in the main text. The density profile was solved by the conjugated gradient method, which was coded by Hager *et al*..[2, 3] The flow chart and the time cost of the algorithm was shown in figure S1 and S2, respectively.

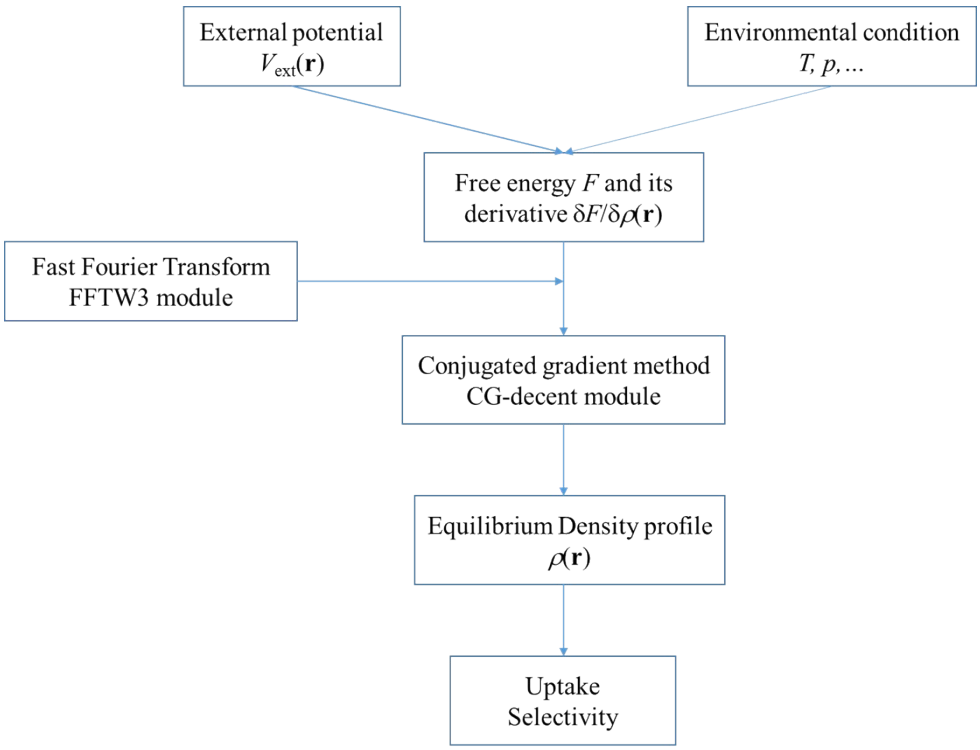

Figure S1 Flow chart of the CDFT algorithm

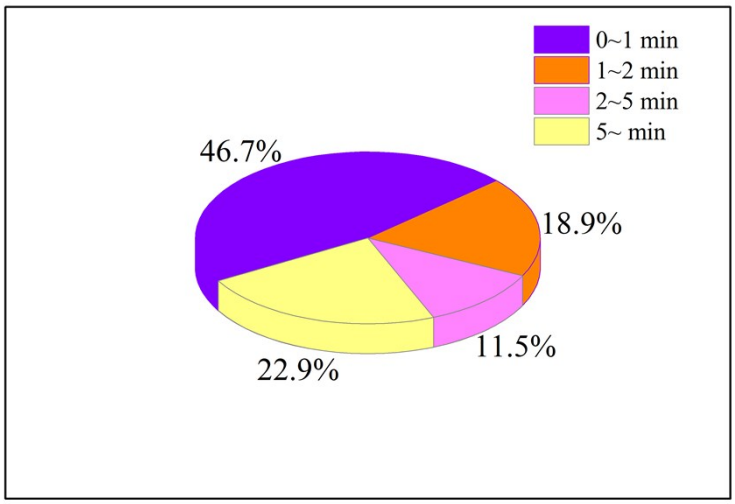

Figure S2 Time cost of the CDFT calculation.

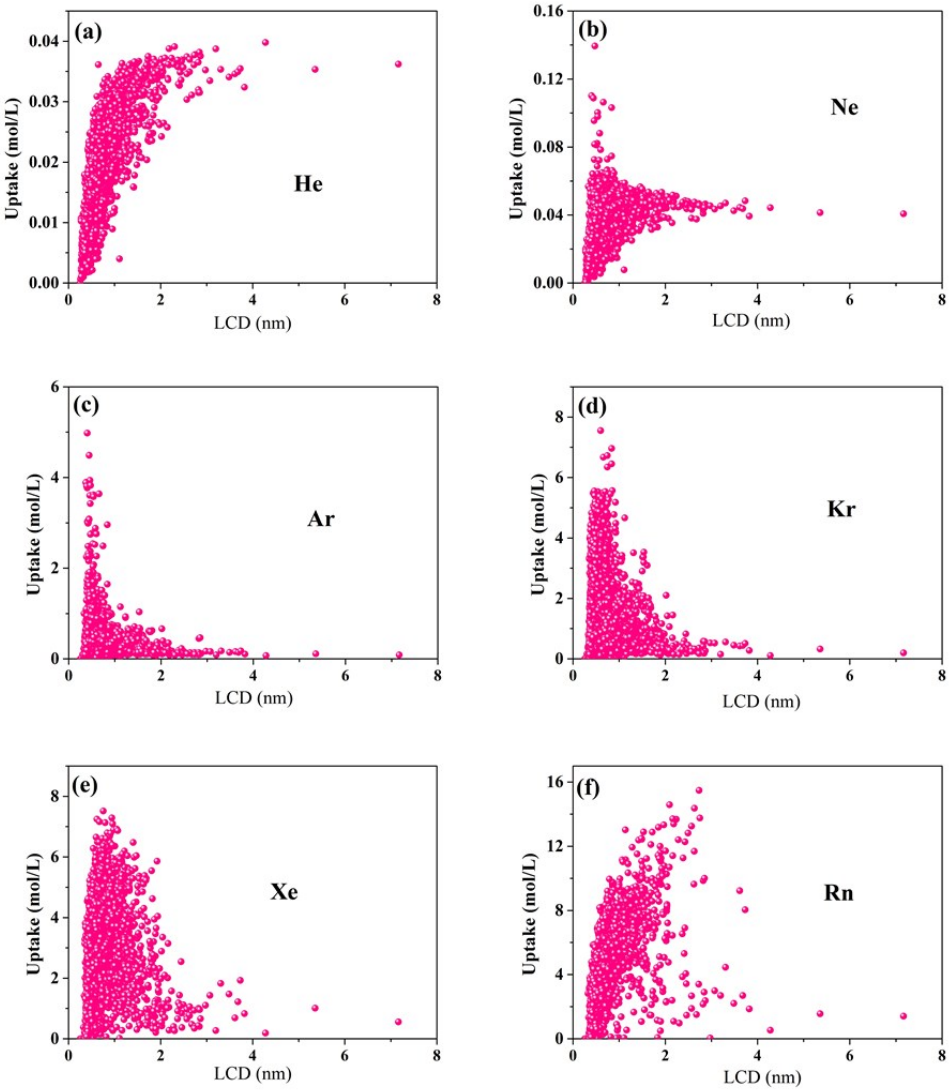

Figure S3. Correlations between the uptake and largest cavity diameter (LCD) of the adsorbents.

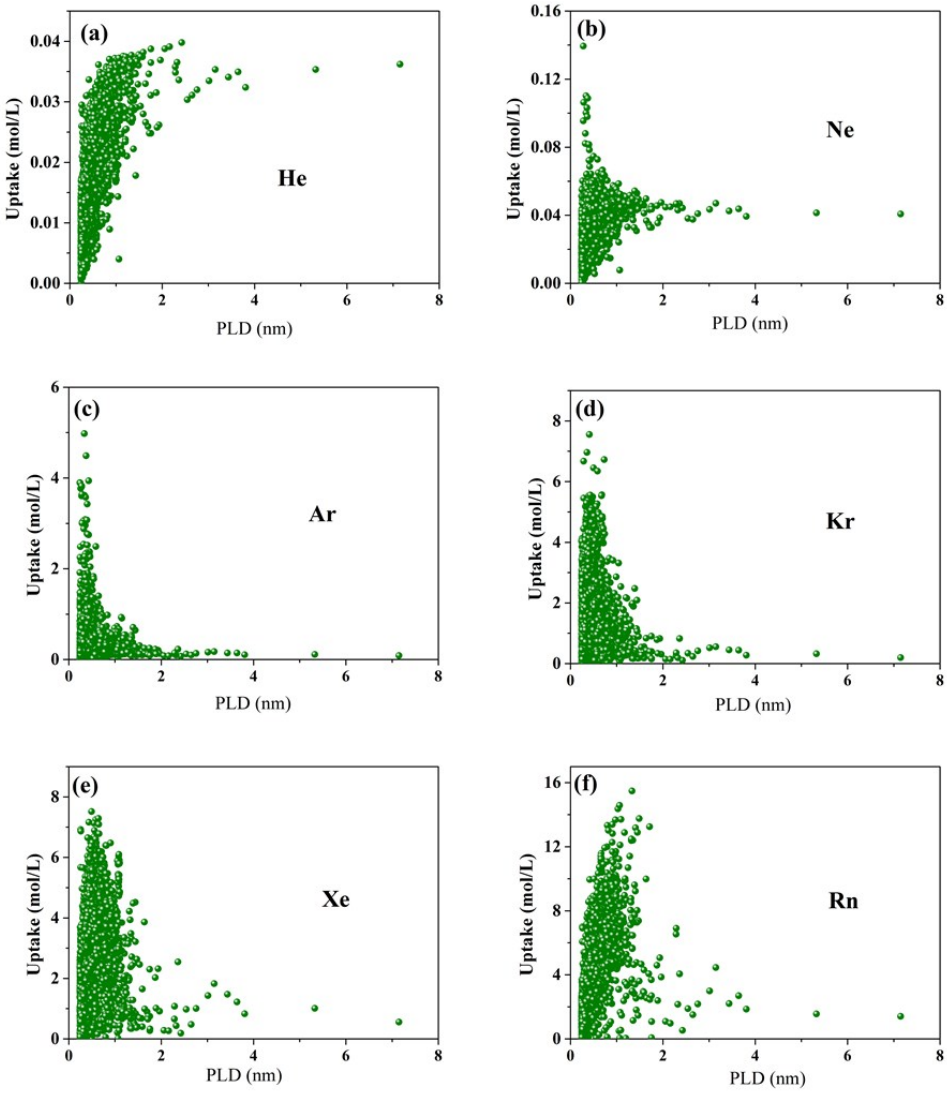

Figure S4. Correlations between the uptake and pore limit diameter (PLD) of the adsorbents.

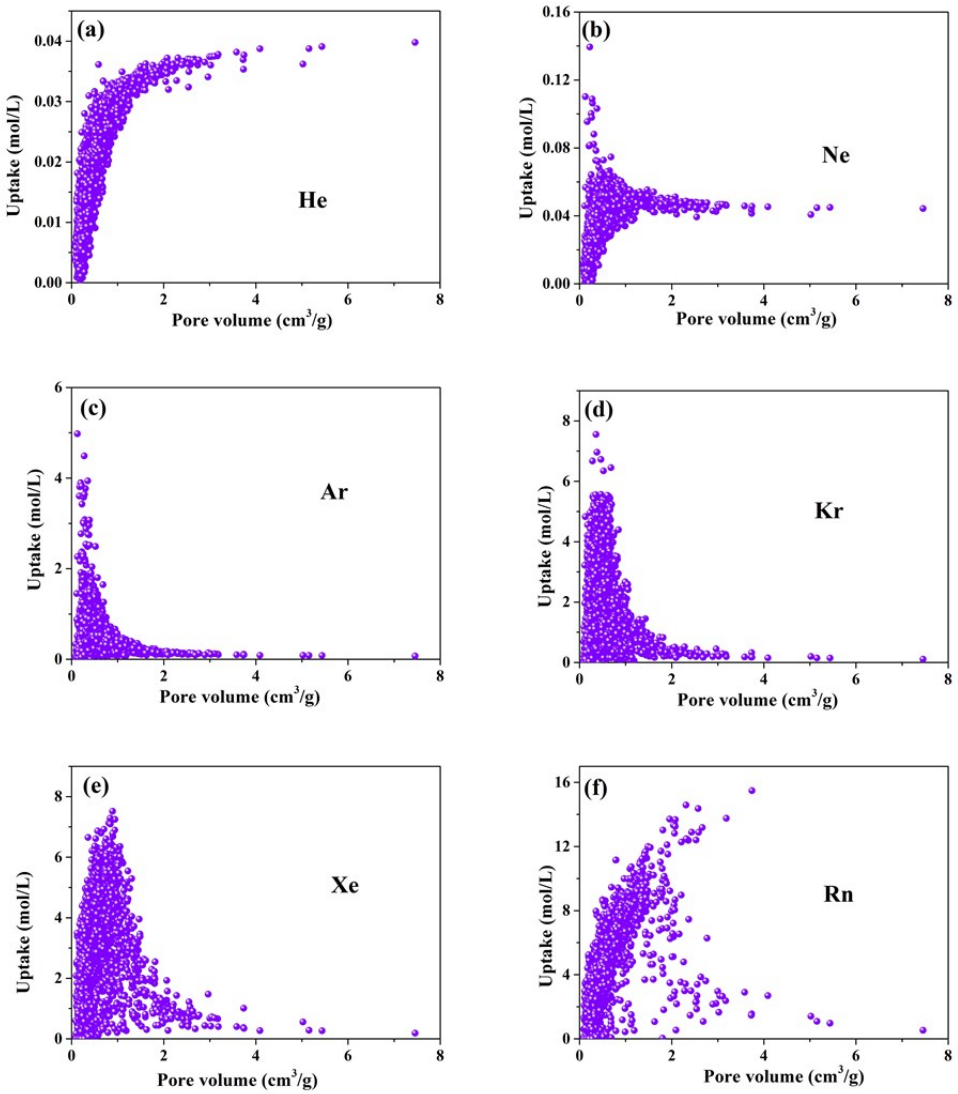

Figure S5. Correlations between the uptake and void fraction of the adsorbents.

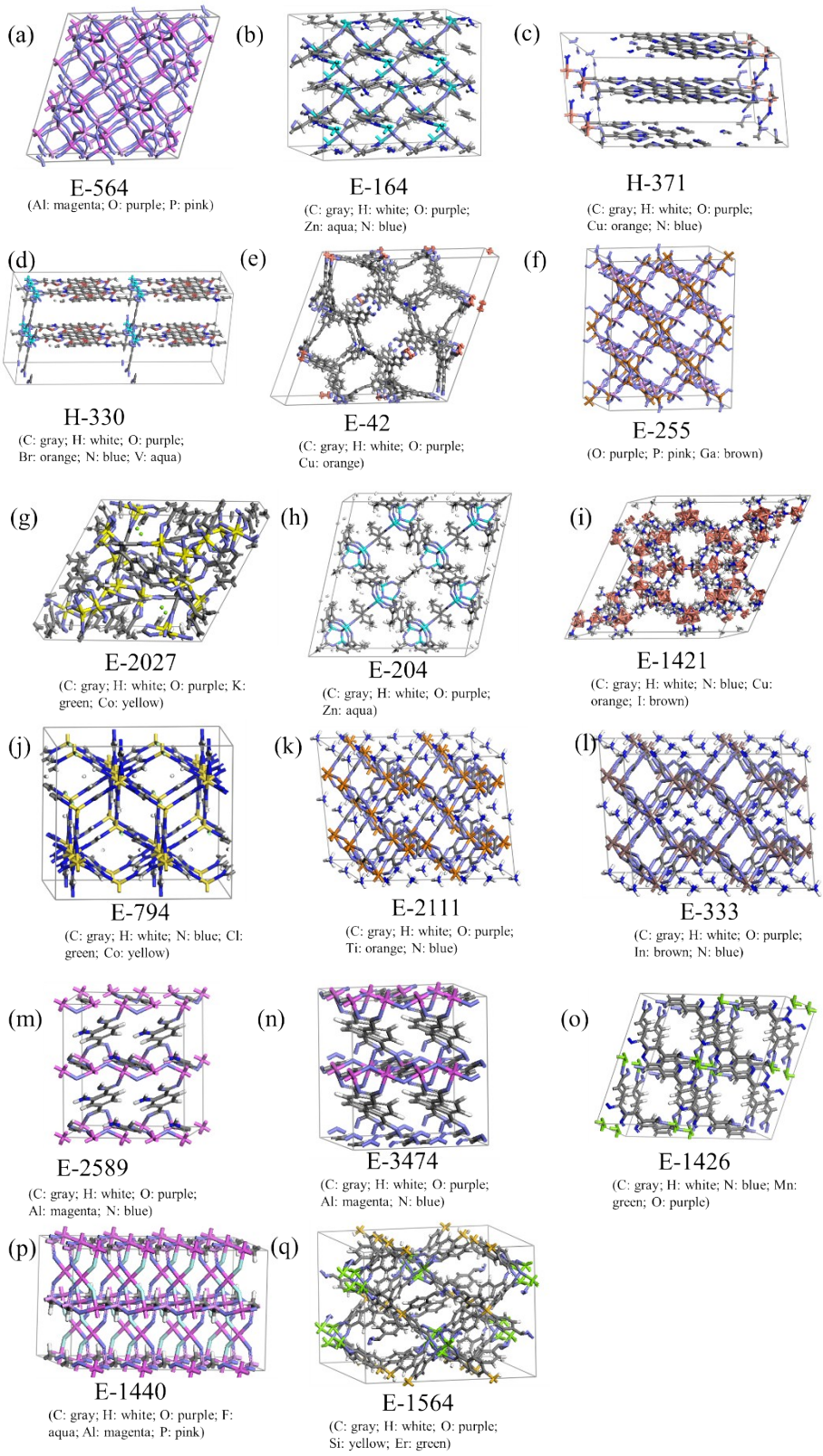

Figure S6. The structures of the most favorable separation adsorbents.

dynamic configuration of E-42 in the MD simulation:

In file “E-42.mp4”