Supporting Information for

“Two-Dimensional Icy Water Clusters Between a Pair of Graphene-Like Molecules or Graphene Sheets”

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1. Geometry and Energy of \((\text{H}_2\text{O})_{1,2}\) as the inter-layer separation of coronene pair is varied.

1-1. Cor/(\text{H}_2\text{O})_1/Cor 
1-2. Cor/(\text{H}_2\text{O})_2/Cor (Starting from dHdd conformer) 
1-3. Cor/(\text{H}_2\text{O})_2/Cor (Starting from uHdd conformer)

Calculation method: SCC-DFTB-3D

Interaction energy of water clusters is defined as;

\[
\begin{align*}
E_1 &= E_{\text{total}} - 2 \times E_{\text{sub}} - n \times E_{\text{water}} \\
E_2 &= E_1 - E_{\text{sub-sub}}
\end{align*}
\]

where \(E_{\text{total}}\), \(E_{\text{sub}}\), \(E_{\text{water}}\), \(E_{\text{sub-sub}}\) are the total energy of cluster, energy of a single water, energy of the substrate, and energy of the substrate pair, respectively
1-1. Cor/(H$_2$O)/Cor

At $(d_x, d_y, d_z) = (0,0,15)$ Å

$E_1 = -2.82$ kcal/mol

$E_2 = -2.83$ kcal/mol

**Figure S1.** Interaction energy as a function of the Cor-Cor distance ($d_z$) for (H$_2$O)$_1$ between a pair of sandwiched Cors (left) and geometry at $(d_x,d_y,d_z) = (0,0,15)$ Å (right).
At $(d_x, d_y, d_z) = (0, 0, 5.9) \text{ Å}$

$E_1 = -5.53 \text{ kcal/mol}$

$E_2 = -3.76 \text{ kcal/mol (minimum)}$

**Figure S2.** Interaction energy as a function of the Cor-Cor distance ($d_z$) for $(\text{H}_2\text{O})_1$ between a pair of sandwiched Cors (left) and geometry at $(d_x, d_y, d_z) = (0, 0, 5.9) \text{ Å}$ (right).
Figure S3. Interaction energy as a function of the Cor-Cor distance ($d_z$) for (H$_2$O)$_1$ between a pair of sandwichedCors (left) and geometry at ($d_x, d_y, d_z$) = (0,0,5.0) Å (right).
1-2. Cor/(H₂O)₂/Cor (Starting from dHdd conformer)

At \((d_x, d_y, d_z) = (0,0,15) \text{ Å}\)

\[
\begin{align*}
E_1 &= -9.65 \text{ kcal/mol} \\
E_2 &= -9.66 \text{ kcal/mol}
\end{align*}
\]

Figure S4. Interaction energy as a function of the Cor-Cor distance \((d_z)\) for \((\text{H}_2\text{O})_2\) (starting from dHdd conformer) between a pair of sandwiched Cors (left) and geometry at \((d_x, d_y, d_z) = (0,0,15) \text{ Å}\) (right).
Figure S5. Interaction energy as a function of the Cor-Cor distance ($d_z$) for (H$_2$O)$_2$ (starting from dHdd conformer) between a pair of sandwichedCors (left) and geometry at ($d_x,d_y,d_z$) = (0,0,7.5) Å (right).
At \( (d_x, d_y, d_z) = (0,0,6.2) \) Å

\[
E_1 = -13.9 \text{ kcal/mol} \\
E_2 = -12.6 \text{ kcal/mol (minimum)}
\]

**Figure S6.** Interaction energy as a function of the Cor-Cor distance \( (d_z) \) for \((\text{H}_2\text{O})_2\) (starting from dHdd conformer) between a pair of sandwiched Cors (left) and geometry at \((d_x,d_y,d_z) = (0,0,6.2) \) Å (right).
At \((d_x, d_y, d_z) = (0,0,5.6) \text{ Å}\)

\[ E_1 = -14.7 \text{ kcal/mol (minimum)} \]
\[ E_2 = -12.4 \text{ kcal/mol} \]

**Figure S7.** Interaction energy as a function of the Cor-Cor distance \(d_z\) for \((\text{H}_2\text{O})_2\) (starting from dHdd conformer) between a pair of sandwiched Cors (left) and geometry at \((d_x, d_y, d_z) = (0,0,5.6) \text{ Å}\) (right).
1-3. Cor/(H₂O)₂/Cor (Starting from uHdd conformer)

At \((d_x, d_y, d_z) = (0,0,15) \, \text{Å}\)

\(E_1 = -9.27 \, \text{kcal/mol}\)
\(E_2 = -9.28 \, \text{kcal/mol}\)

Figure S8. Interaction energy as a function of the Cor-Cor distance \(d_z\) for \((\text{H}_2\text{O})_2\) (starting from uHdd conformer) between a pair of sandwiched Cors (left) and geometry at \((d_x, d_y, d_z) = (0,0,15) \, \text{Å}\) (right).
Figure S9. Interaction energy as a function of the Cor-Cor distance \((d_z)\) for \((\text{H}_2\text{O})_2\) (starting from uHdd conformer) between a pair of sandwiched Cors (left) and geometry at \((d_x,d_y,d_z) = (0,0,8.0)\) Å (right).
Figure S10. Interaction energy as a function of the Cor-Cor distance ($d_z$) for (H$_2$O)$_2$ (starting from uHdd conformer) between a pair of sandwiched Cors (left) and geometry at ($d_x$,$d_y$,$d_z$) = (0,0,6.3) Å (right).

At ($d_x$,$d_y$,$d_z$) = (0,0,6.3) Å

$E_1 = -13.8$ kcal/mol

$E_2 = -12.6$ kcal/mol (minimum)
At \((d_x,d_y,d_z) = (0,0,5.6)\,\text{Å}\)

\[E_1 = -14.7\,\text{kcal/mol (minimum)}\]

\[E_2 = -12.4\,\text{kcal/mol}\]

**Figure S11.** Interaction energy as a function of the Cor-Cor distance \((d_z)\) for \((\text{H}_2\text{O})_2\) (starting from uHdd conformer) between a pair of sandwiched Cors (left) and geometry at \((d_x,d_y,d_z) = (0,0,5.6)\,\text{Å}\) (right).
At \((d_x, d_y, d_z) = (0, 0, 5.6) \text{ Å}\)
\[E_1 = -14.7 \text{ kcal/mol}\]

At \((d_x, d_y, d_z) = (-0.4, -0.3, 5.6) \text{ Å}\)
\[E_1 = -14.9 \text{ kcal/mol}\]

**Figure S12.** Geometry change of \((\text{H}_2\text{O})_2\) as one Cor plane is laterally displaced from the other.
2. Geometry and Energy of \((\text{H}_2\text{O})_{3.5}\) as the inter-layer separation of coronene pair is varied.

2-1. Cor/(\text{H}_2\text{O})_3/Cor
2-2. Cor/(\text{H}_2\text{O})_4/Cor (Starting from dHdd conformer)
2-3. Cor/(\text{H}_2\text{O})_5/Cor (Starting from uHdd conformer)

Calculation method: SCC-DFTB-3D

In order to assess the ring structure, the following parameters are calculated.

\[ <z> = \frac{1}{n} \sum_{i=1}^{n} z_{Oi} \] : Mean distance of oxygen atoms \((z_{Oi})\) of water cluster ring from the bottom substrate.

\[ \sigma_z = \sqrt{\frac{1}{n} \sum_{i=1}^{n} (z_{Oi} - <z>)^2} \] : Deviation of \(z_{Oi}\) from the mean value \(<z>\). This parameter indicates the flatness of the water cluster ring.

\[ \text{FF} = \sqrt{\frac{1}{n} \sum_{i=1}^{n} [(x_{Oi} - X_i)^2 + (y_{Oi} - Y_i)^2]} \] : Geometry fit factor, where \((x_{Oi}, y_{Oi})\) is the coordinate of \(i\)-th oxygen in the water cluster ring and \((X_i, Y_i)\) is that in an ideal ring geometry, i.e. equilateral triangle for \(n = 3\), square for \(n = 4\), regular pentagon for \(n = 5\), regular hexagon for \(n = 6\).
2-1. **Cor/(H$_2$O)$_3$/Cor**

At $(d_x,d_y,d_z)=(0,0,15)$ Å

$E_1 = -14.7$ kcal/mol, $E_2 = -12.4$ kcal/mol

$<z>=3.07$ Å, $\sigma_z=0.01$ Å, FF=0.002 Å

**Figure S13.** Interaction energy ($E_1$) and geometry parameters ($<z>$, $\sigma_z$, FF) as a function of the Cor-Cor distance ($d_z$) for (H$_2$O)$_3$ between a pair of sandwichedCors (left) and the geometry at $(d_x,d_y,d_z)=(0,0,15)$ Å (right).
At \((d_x,d_y,d_z)=(0,0,8.0)\) Å

\[ E_1 = -23.8 \text{ kcal/mol}, \quad E_2 = -23.5 \text{ kcal/mol} \]

\(<z>=3.71 \text{ Å}, \quad \sigma_z=0.73 \text{ Å}, \quad \text{FF}=0.20 \text{ Å} \)

**Figure S14.** Interaction energy \((E_1)\) and geometry parameters \((<z>, \sigma_z, \text{FF})\) as a function of the Cor-Cor distance \((d_z)\) for \((\text{H}_2\text{O})_3\) between a pair of sandwiched Cors (left) and the geometry at \((d_x,d_y,d_z)=(0,0,8.0)\) Å (right).
At \((d_x, d_y, d_z) = (0,0,6.3) \text{ Å}\)

\[E_1 = -27.1 \text{ kcal/mol}, \ E_2 = -25.9 \text{ kcal/mol}\]

\(<z> = 3.13 \text{ Å}, \ \sigma_z = 0.04 \text{ Å}, \ \text{FF}=0.001 \text{ Å}\)

**Figure S15.** Interaction energy \((E_1)\) and geometry parameters \(<z>, \ \sigma_z, \ \text{FF}\) as a function of the Cor-Cor distance \(d_z\) for \((\text{H}_2\text{O})_3\) between a pair of sandwiched Cors (left) and the geometry at \((d_x, d_y, d_z) = (0,0,6.3) \text{ Å}\) (right).
At \((d_x, d_y, d_z) = (0,0,6.1)\) Å

E_1 = -27.3 kcal/mol, E_2 = -25.8 kcal/mol

\(<z> = 3.04\) Å, \(\sigma_z = 0.03\) Å, FF=0.002 Å

**Figure S16.** Interaction energy (\(E_1\)) and geometry parameters (\(<z>, \sigma_z, FF\)) as a function of the Cor-Cor distance \((d_z)\) for \((H_2O)_3\) between a pair of sandwiched Cors (left) and the geometry at \((d_x, d_y, d_z) = (0,0,6.1)\) Å (right).
Figure S17. Geometry change of (H$_2$O)$_3$ as one Cor plane is laterally displaced from the other.
2-2. Cor/(H₂O)₄/Cor

At \((d_x, d_y, d_z) = (0,0,15) \text{ Å}\)

\[ E_1 = -34.2 \text{ kcal/mol}, \quad E_2 = -34.2 \text{ kcal/mol} \]

\(<z>=3.18 \text{ Å}, \quad \sigma_z=0.07 \text{ Å}, \quad \text{FF}=0.04 \text{ Å}\)

**Figure S18.** Interaction energy \((E_i)\) and geometry parameters \(<z>, \sigma_z, \text{FF}\) as a function of the Cor-Cor distance \(d_z\) for \((H₂O)_4\) between a pair of sandwiched Cors (left) and the geometry at \((d_x,d_y,d_z) = (0,0,15) \text{ Å}\) (right).
At \((d_x, d_y, d_z) = (0,0,8.5) \text{ Å}\)

\[ E_1 = -35.5 \text{ kcal/mol}, \quad E_2 = -35.2 \text{ kcal/mol} \]

\(<z> = 3.38 \text{ Å}, \quad \sigma_z = 0.23 \text{ Å}, \quad \text{FF} = 0.01 \text{ Å} \]

**Figure S19.** Interaction energy (\(E_1\)) and geometry parameters (\(<z>, \sigma_z, \text{FF}\)) as a function of the Cor-Cor distance \((d_z)\) for \((\text{H}_2\text{O})_4\) between a pair of sandwichedCors (left) and the geometry at \((d_x, d_y, d_z) = (0,0,8.5) \text{ Å}\) (right).
Figure S20. Interaction energy ($E_1$) and geometry parameters ($\langle z \rangle$, $\sigma_z$, FF) as a function of the Cor-Cor distance ($d_z$) for (H$_2$O)$_4$ between a pair of sandwiched Cors (left) and the geometry at ($d_x, d_y, d_z$) = (0,0,7.0) Å (right).
At \((d_x,d_y,d_z)=(0,0,6.2)\) Å

\[ E_1 = -41.8 \text{ kcal/mol, } E_2 = -40.4 \text{ kcal/mol} \]

\(<z>=3.14 \text{ Å, } \sigma_z=0.05 \text{ Å, FF}=0.01 \text{ Å}\)

**Figure S21.** Interaction energy \((E_1)\) and geometry parameters \((<z>, \sigma_z, \text{ FF})\) as a function of the Cor-Cor distance \((d_z)\) for \((H_2O)_4\) between a pair of sandwiched Cors (left) and the geometry at \((d_x,d_y,d_z)=(0,0,6.2)\) Å (right).
Figure S22. Geometry change of $(\text{H}_2\text{O})_4$ as one Cor plane is laterally displaced from the other.
2-3. Cor/(H$_2$O)$_5$/Cor

At $(d_x,d_y,d_z) = (0,0,15)$ Å

$E_1 = -44.9$ kcal/mol, $E_2 = -44.9$ kcal/mol

$<z> = 3.18$ Å, $\sigma_z = 0.16$ Å, FF=0.04 Å

**Figure S23.** Interaction energy ($E_1$) and geometry parameters ($<z>$, $\sigma_z$, FF) as a function of the Cor-Cor distance ($d_z$) for (H$_2$O)$_5$ between a pair of sandwiched Cors (left) and the geometry at $(d_x,d_y,d_z) = (0,0,15)$ Å (right).
At \((d_x, d_y, d_z) = (0,0,8.0)\) Å

\[
\begin{align*}
E_1 &= -48.0 \text{ kcal/mol}, \quad E_2 = -47.7 \text{ kcal/mol} \\
\langle z \rangle &= 3.61 \text{ Å}, \quad \sigma_z = 0.55 \text{ Å}, \quad \text{FF} = 0.11 \text{ Å}
\end{align*}
\]

**Figure S24.** Interaction energy \((E_1)\) and geometry parameters \((\langle z \rangle, \sigma_z, \text{FF})\) as a function of the Cor-Cor distance \((d_z)\) for \((H_2O)_5\) between a pair of sandwiched Cors (left) and the geometry at \((d_x, d_y, d_z) = (0,0,8.0)\) Å (right).
At \((d_x, d_y, d_z) = (0,0,6.3)\) Å

\[ E_1 = -53.3\text{ kcal/mol}, \quad E_2 = -52.1\text{ kcal/mol} \]

\[ \langle z \rangle = 3.14\text{ Å}, \quad \sigma_z = 0.11\text{ Å}, \quad \text{FF} = 0.02\text{ Å} \]

**Figure S25.** Interaction energy (\(E_1\)) and geometry parameters (\(\langle z \rangle, \sigma_z, \text{FF}\)) as a function of the Cor-Cor distance \((d_z)\) for \((\text{H}_2\text{O})_5\) between a pair of sandwiched Cors (left) and the geometry at \((d_x,d_y,d_z) = (0,0,6.3)\) Å (right).
At \((d_x, d_y, d_z) = (0,0,6.3) \text{ Å}\) 
\[ E_1 = -41.8 \text{ kcal/mol} \]

At \((d_x, d_y, d_z) = (-0.4,-0.5,6.3) \text{ Å}\) 
\[ E_1 = -42.0 \text{ kcal/mol} \]

**Figure S26.** Geometry change of \((\text{H}_2\text{O})_5\) as one Cor plane is laterally displaced from the other.
3. Geometry and Energy of (H₂O)₆ as the inter-layer separation of coronene pair is varied.

3-1. Cor/(H₂O)₆ (ring)/Cor
3-2. Cor/(H₂O)₆ (book)/Cor
3-3. Cor/(H₂O)₆ (bag)/Cor
3-4. Cor/(H₂O)₆ (cage)/Cor
3-5. Cor/(H₂O)₆ (prism)/Cor

Calculation method: SCC-DFTB-3D
3-1. Cor/(H$_2$O)$_6$(ring)/Cor

At $(d_x, d_y, d_z) = (0,0,15)$ Å

$E_1 = -54.2$ kcal/mol, $E_2 = -54.2$ kcal/mol

$\langle z \rangle = 3.28$ Å, $\sigma_z = 0.22$ Å, FF = 0.02 Å

**Figure S27.** Interaction energy ($E_1$) and geometry parameters ($\langle z \rangle$, $\sigma_z$, FF) as a function of the Cor-Cor distance ($d_z$) for (H$_2$O)$_6$ (ring) between a pair of sandwiched Cors (left) and the geometry at $(d_x, d_y, d_z) = (0,0,15)$ Å (right).
At \( (d_x,d_y,d_z) = (0,0,8.0) \text{ Å} \)

\[ E_1 = -57.9 \text{ kcal/mol}, \ E_2 = -57.6 \text{ kcal/mol} \]

\(<z>=3.56 \text{ Å}, \ \sigma_z=0.42 \text{ Å}, \ FF=0.03 \text{ Å} \)

**Figure S28.** Interaction energy (\( E_1 \)) and geometry parameters \(<z>, \ \sigma_z, \ FF \) as a function of the Cor-Cor distance \( (d_z) \) for \((\text{H}_2\text{O})_6 \text{ (ring)} \) between a pair of sandwiched Cors (left) and the geometry at \((d_x,d_y,d_z) = (0,0,8.0) \text{ Å} \) (right).
At \((d_x,d_y,d_z) = (0,0,6.5)\) Å

\[ E_1 = -64.5 \text{ kcal/mol}, \ E_2 = -63.4 \text{ kcal/mol} \]

\(<z> = 3.25 \text{ Å}, \ \sigma_z = 0.20 \text{ Å}, \ FF = 0.006 \text{ Å} \]

**Figure S29.** Interaction energy \(E_1\) and geometry parameters \(<z>, \ \sigma_z, \ FF\) as a function of the Cor-Cor distance \(d_z\) for \((H_2O)_6\) (ring) between a pair of sandwiched Cors (left) and the geometry at \((d_x,d_y,d_z) = (0,0,6.5)\) Å (right).
3-2. Cor/(H₂O)$_6$ (book)/Cor

At $(d_x,d_y,d_z) = (0,0,15)$ Å

$E_1 = -55.2$ kcal/mol,
$E_2 = -55.2$ kcal/mol

Figure S30. Interaction energy ($E_1$) as a function of the Cor-Cor distance ($d_z$) for (H₂O)$_6$ (book) between a pair of sandwiched Cors (left) and the geometry at $(d_x,d_y,d_z) = (0,0,15)$ Å (right).
At \((d_x, d_y, d_z) = (0, 0, 8.0) \text{ Å}\)

\[E_1 = -59.7 \text{ kcal/mol},\]
\[E_2 = -59.4 \text{ kcal/mol}\]

**Figure S31.** Interaction energy \((E_1)\) as a function of the Cor-Cor distance \((d_z)\) for \((\text{H}_2\text{O})_6\) (book) between a pair of sandwiched Cors (left) and the geometry at \((d_x, d_y, d_z) = (0, 0, 8.0) \text{ Å}\) (right).
At \((d_{x}, d_{y}, d_{z}) = (0,0,6.5) \text{ Å}\)

\[ E_{1} = -64.8 \text{ kcal/mol}, \]
\[ E_{2} = -53.7 \text{ kcal/mol} \]

**Figure S32.** Interaction energy \(E_{1}\) as a function of the Cor-Cor distance \(d_{z}\) for \((\text{H}_2\text{O})_6\) (book) between a pair of sandwiched Cors (left) and the geometry at \((d_{x}, d_{y}, d_{z}) = (0,0,6.5) \text{ Å}\) (right).
3-3. Cor/(H$_2$O)$_6$ (bag)/Cor

At ($d_x, d_y, d_z$) = (0,0,15) Å

$E_1 = -53.3$ kcal/mol,
$E_2 = -53.3$ kcal/mol

**Figure S33.** Interaction energy ($E_1$) as a function of the Cor-Cor distance ($d_z$) for (H$_2$O)$_6$ (bag) between a pair of sandwiched Cors (left) and the geometry at ($d_x, d_y, d_z$) = (0,0,15) Å (right).
At \((d_x,d_y,d_z) = (0,0,8.5) \text{ Å}\)

\[E_1 = -57.9 \text{ kcal/mol},\]
\[E_2 = -57.7 \text{ kcal/mol}\]

**Figure S34.** Interaction energy \((E_1)\) as a function of the Cor-Cor distance \((d_z)\) for \((\text{H}_2\text{O})_6\) (bag) between a pair of sandwiched Cors (left) and the geometry at \((d_x,d_y,d_z) = (0,0,8.5) \text{ Å}\) (right).
At \((d_x,d_y,d_z)=(0,0,7.5) \text{ Å}\)

\[E_1 = -53.8 \text{ kcal/mol}, \]
\[E_2 = -53.3 \text{ kcal/mol}\]

**Figure S35.** Interaction energy \((E_1)\) as a function of the Cor-Cor distance \((d_z)\) for \((\text{H}_2\text{O})_6\) (bag) between a pair of sandwiched Cors (left) and the geometry at \((d_x,d_y,d_z)=(0,0,7.5) \text{ Å}\) (right).
At \((d_x, d_y, d_z) = (0,0,7.0) \text{ Å}\)

\[ E_1 = -60.7 \text{ kcal/mol}, \]
\[ E_2 = -60.0 \text{ kcal/mol} \]

**Figure S36.** Interaction energy \((E_1)\) as a function of the Cor-Cor distance \((d_z)\) for \((\text{H}_2\text{O})_6 \text{ (bag)}\) between a pair of sandwiched Cors (left) and the geometry at \((d_x,d_y,d_z) = (0,0,7.0) \text{ Å} \) (right).
At \((d_x, d_y, d_z) = (0, 0, 6.4) \text{ Å}\)

\[ E_1 = -63.1 \text{ kcal/mol}, \]
\[ E_2 = -62.0 \text{ kcal/mol} \]

**Figure S37.** Interaction energy \((E_1)\) as a function of the Cor-Cor distance \(d_z\) for \((\text{H}_2\text{O})_6\) (bag) between a pair of sandwiched Cors (left) and the geometry at \((d_x, d_y, d_z) = (0, 0, 6.4) \text{ Å}\) (right).
Figure S38. Geometry change of (H₂O)₆ (bag) as one Cor plane is laterally displaced from the other.

At \((d_x, d_y, d_z) = (0, 0, 6.4) \text{ Å}\)

\[ E_1 = -63.1 \text{ kcal/mol} \]  

At \((d_x, d_y, d_z) = (0.4, 0, 6.4) \text{ Å}\)

\[ E_1 = -63.2 \text{ kcal/mol} \]
3-4. Cor/(H₂O)₆(cage)/Cor

At \((d_x, d_y, d_z) = (0,0,15) \, \text{Å}\)

\[
E_1 = -54.3 \, \text{kcal/mol}, \\
E_2 = -54.3 \, \text{kcal/mol}
\]

**Figure S39.** Interaction energy \((E_1)\) as a function of the Cor-Cor distance \((d_z)\) for \((H₂O)_₆\) (cage) between a pair of sandwiched Cors (left) and the geometry at \((d_x, d_y, d_z) = (0,0,15) \, \text{Å}\) (right).
At $(d_x, d_y, d_z) = (0,0,8.5) \text{Å}$

$E_1 = -59.3 \text{ kcal/mol}$,
$E_2 = -59.0 \text{ kcal/mol}$

**Figure S40.** Interaction energy ($E_1$) as a function of the Cor-Cor distance ($d_z$) for $(\text{H}_2\text{O})_6$ (cage) between a pair of sandwiched Cors (left) and the geometry at $(d_x, d_y, d_z) = (0,0,8.5) \text{Å}$ (right).
At \((d_x, d_y, d_z) = (0, 0, 7.5) \, \text{Å}\)

\[ \begin{align*}
E_1 &= -57.6 \, \text{kcal/mol}, \\
E_2 &= -57.2 \, \text{kcal/mol}
\end{align*} \]

**Figure S41.** Interaction energy \((E_1)\) as a function of the Cor-Cor distance \((d_z)\) for \((\text{H}_2\text{O})_6\) (cage) between a pair of sandwiched Cors (left) and the geometry at \((d_x, d_y, d_z) = (0,0,7.5) \, \text{Å}\) (right).
At \((d_x, d_y, d_z) = (0, 0, 7.0)\) Å

\[
E_1 = -61.2 \text{ kcal/mol}, \\
E_2 = -60.5 \text{ kcal/mol}
\]

**Figure S42.** Interaction energy \((E_1)\) as a function of the Cor-Cor distance \((d_z)\) for \((\text{H}_2\text{O})_6\) (cage) between a pair of sandwiched Cors (left) and the geometry at \((d_x, d_y, d_z) = (0, 0, 7.0)\) Å (right).
At \((d_x, d_y, d_z) = (0, 0, 6.4)\) Å

\[
\begin{align*}
E_1 &= -62.2 \text{ kcal/mol}, \\
E_2 &= -61.1 \text{ kcal/mol}
\end{align*}
\]

**Figure S43.** Interaction energy \((E_1)\) as a function of the Cor-Cor distance \((d_z)\) for \((H_2O)_6\) (cage) between a pair of sandwiched Cors (left) and the geometry at \((d_x,d_y,d_z) = (0,0,6.4)\) Å (right).
3-5. Cor/(H$_2$O)$_6$ (prism)/Cor

At $(d_x, d_y, d_z) = (0,0,15)$ Å

$E_1 = -52.6$ kcal/mol,  
$E_2 = -52.6$ kcal/mol

**Figure S44.** Interaction energy ($E_1$) as a function of the Cor-Cor distance ($d_z$) for (H$_2$O)$_6$ (prism) between a pair of sandwiched Cors (left) and the geometry at $(d_x,d_y,d_z) = (0,0,15)$ Å (right).
At $(d_x, d_y, d_z) = (0, 0, 9.0) \text{ Å}$

$E_1 = -52.4 \text{ kcal/mol}$,
$E_2 = -52.2 \text{ kcal/mol}$

**Figure S45.** Interaction energy ($E_1$) as a function of the Cor-Cor distance ($d_z$) for $(\text{H}_2\text{O})_6$ (prism) between a pair of sandwiched Cors (left) and the geometry at $(d_x, d_y, d_z) = (0, 0, 9.0) \text{ Å}$ (right).
At \((d_x, d_y, d_z) = (0, 0, 7.5) \text{Å}\)

\[
E_1 = -54.6 \text{ kcal/mol}, \\
E_2 = -54.1 \text{ kcal/mol}
\]

**Figure S46.** Interaction energy \((E_1)\) as a function of the Cor-Cor distance \((d_z)\) for \((\text{H}_2\text{O})_6\) (prism) between a pair of sandwichedCors (left) and the geometry at \((d_x, d_y, d_z) = (0, 0, 7.5) \text{Å}\) (right).
At $(d_x,d_y,d_z)= (0,0,6.5) \text{ Å}$

$E_1 = -64.9 \text{ kcal/mol}$,
$E_2 = -63.8 \text{ kcal/mol}$

**Figure S47.** Interaction energy ($E_1$) as a function of the Cor-Cor distance ($d_z$) for (H$_2$O)$_6$ (prism) between a pair of sandwiched Cors (left) and the geometry at $(d_x,d_y,d_z) = (0,0,6.5) \text{ Å}$ (right).
4. Many body Interaction of (H_2O)_{2-4} clusters extracted from substrates of this study

$\Delta E_w$: Total interaction energy

$E_{\text{def}}$: deformation of energy of monomers, $E^{(2)}$: two-body interaction energy,

$E^{(3)}$: three-body interaction energy, $E^{(4)}$: four-body interaction energy.

All values are in kcal/mol

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