*Supplementary Information for:*

# Computational screening of functional groups for capture of toxic industrial chemicals in porous materials

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**Table S1**: Binding energies at 0 K in kJ/mol of toxic industrial chemicals ($BE_{TIC}$) and water ($BE_{H2O}$) with ten functional group candidates. The five values for each case are from five different starting configurations. The last column represents the difference between the lowest binding energy of water and the lowest binding energy of the toxic industrial chemical for each case. A positive value indicates that the binding of the toxic industrial chemical is stronger than that of water.

| **Functional group** | $BE_{H2SO4}$ | $BE_{H2O}$ | **Lowest *BE* of $H_2O$ – Lowest *BE* of $H_2SO_4$** |
|---|---|---|---|
| R-COOCu | -183.8, -183.8, -51.6, -30.7, 118.6 | -97.8, -97.8, -97.8, -10.8, -10.7 | 86.0 |
| R-COOAg | -94.1, -93.4, -34.4, -32.8, 331.5 | -51.5, -51.5, -51.4, -48.3, -12.3 | 42.6 |
| R-COOLi | -112.8, -112.1, -105.3, -62.5, -57.4 | -70.2, -70.1, -68.3, -11.9, -11.8 | 42.6 |
| R-P(=O)$(OH)_2$ | -82.1, -78.3, -78.2, -74.8, -17.1 | -42.7, -42.7, -27.7, -15.1, -15.1 | 39.4 |
| R-OP(=O)$(OH)_2$ | -73.6, -53.1, -52.9, -41.4, 267.3 | -44.9, -44.1, -43.7, -43.7, -43.4 | 28.7 |
| R | -34.9, -29.4, -29.4, -22.6, -22.6 | -10.7, -10.6, -6.0, -5.9, -5.3 | 24.3 |
| R-COOH | -59.4, -42.6, -41.3, -35.8, 475.1 | -37.2, -37.2, -37.2, -8.5, -8.4 | 22.2 |
| R-$SO_3H$ | -64.2, -43.5, -33.8, -19.2, 562.2 | -42.7, -42.3, -22.3, -12.7, -11.6 | 21.5 |
| R-$HSO_4$ | -68.3, -63.5, -43.2, -43.1, -41.6 | -46.9, -44.5, -44.5, -44.5, -21.2 | 21.4 |
| R-OOH | -47.5, -44.8, -38.7, -36.0, -35.9 | -27.7, -26.5, -26.4, -13.1, -10.7 | 19.8 |
| R-OH | -46.1, -38.8, -31.6, -28.3, -6.1 | -26.5, -26.5, -16.6, -10.8, -10.8 | 19.6 |

| **Functional group** | $BE_{CO}$ | $BE_{H2O}$ | **Lowest *BE* of $H_2O$ – Lowest *BE* of CO** |
|---|---|---|---|
| R-COOCu | -170.6, -170.5, -170.5, -22.8, -3.1 | -97.8, -97.8, -97.8, -10.8, -10.7 | 72.8 |
| R-COOAg | -49.4, -49.4, -49.4, -6.4, -6.0 | -51.5, -51.5, -51.4, -48.3, -12.3 | -2.1 |
| R | -5.4, -5.4, -5.4, -2.2, -2.2 | -10.7, -10.6, -6.0, -5.9, -5.3 | -5.2 |
| R-OH | -8.7, -6.3, -6.3, -5.6, -4.1 | -26.5, -26.5, -16.6, -10.8, -10.8 | -17.8 |
| R-OOH | -8.2, -8.2, -6.4, -6.2, -3.2 | -27.7, -26.5, -26.4, -13.1, -10.7 | -19.5 |
| R-$HSO_4$ | -20.0, -20.0, -19.8, -10.8, -4.7 | -46.9, -44.5, -44.5, -44.5, -21.2 | -26.9 |
| R-P(=O)$(OH)_2$ | -12.2, -6.0, -5.9, -5.2, -4.8 | -42.7, -42.7, -27.7, -15.1, -15.1 | -30.5 |
| R-$SO_3H$ | -11.6, -7.1, -5.2, -5.1, -4.2 | -42.7, -42.3, -22.3, -12.7, -11.6 | -31.0 |
| R-COOH | -6.1, -5.4, -4.1, -3.9, -3.2 | -37.2, -37.2, -37.2, -8.5, -8.4 | -31.1 |
| R-OP(=O)$(OH)_2$ | -13.0, -13.0, -8.2, -8.2, -4.0 | -44.9, -44.1, -43.7, -43.7, -43.4 | -32.0 |
| R-COOLi | -29.0, -29.0, -29.0, -14.7, -3.1 | -70.2, -70.1, -68.3, -11.9, -11.8 | -41.2 |

| Functional group | $BE_{HCl}$ | $BE_{H2O}$ | Lowest *BE* of $H_2O$ – Lowest *BE* of HCl |
|---|---|---|---|
| R-COOCu | -166.9, -166.9, -56.2, -24.9, -11.5 | -97.8, -97.8, -97.8, -10.8, -10.7 | 69.1 |
| R-COOAg | -87.0, -87.0, -86.6, -20.7, -13.5 | -51.5, -51.5, -51.4, -48.3, -12.3 | 35.4 |
| R-COOLi | -88.4, -88.4, -88.3, -88.3, -12.8 | -70.2, -70.1, -68.3, -11.9, -11.8 | 18.2 |
| R | -11.6, -11.6, -11.6, -10.7, -10.7 | -10.7, -10.6, -6.0, -5.9, -5.3 | 1.0 |
| R-OH | -16.2, -16.0, -11.9, -11.9, -11.8 | -26.5, -26.5, -16.6, -10.8, -10.8 | -10.3 |
| R-OOH | -16.7, -16.0, -13.4, -13.4, -10.3 | -27.7, -26.5, -26.4, -13.1, -10.7 | -11.0 |
| R-P(=O)$(OH)_2$ | -28.6, -27.4, -16.0, -15.3, -11.0 | -42.7, -42.7, -27.7, -15.1, -15.1 | -14.1 |
| R-COOH | -19.2, -19.0, -19.0, -11.0, -8.9 | -37.2, -37.2, -37.2, -8.5, -8.4 | -18.0 |
| R-OP(=O)$(OH)_2$ | -25.4, -25.3, -23.0, -16.7, -11.3 | -44.9, -44.1, -43.7, -43.7, -43.4 | -19.6 |
| R-$SO_3H$ | -19.5, -19.5, -19.5, -13.1, -13.0 | -42.7, -42.3, -22.3, -12.7, -11.6 | -23.2 |
| R-$HSO_4$ | -19.6, -19.6, -19.1, -13.5, -13.5 | -46.9, -44.5, -44.5, -44.5, -21.2 | -27.3 |

| Functional group | $BE_{CNCl}$ | $BE_{H2O}$ | Lowest *BE* of $H_2O$ – Lowest *BE* of CNCl |
|---|---|---|---|
| R-COOCu | -142.6, -132.7, -132.7, -132.7, -132.6 | -97.8, -97.8, -97.8, -10.8, -10.7 | 44.9 |
| R-COOAg | -55.3, -55.3, -41.0, -41.0, -33.2 | -51.5, -51.5, -51.4, -48.3, -12.3 | 3.8 |
| R | -12.5, -12.5, -10.8, -10.8, -10.8 | -10.7, -10.6, -6.0, -5.9, -5.3 | 1.8 |
| R-OOH | -26.7, -26.7, -26.7, -13.1, -11.1 | -27.7, -26.5, -26.4, -13.1, -10.7 | -1.0 |
| R-$HSO_4$ | -41.0, -41.0, -41.0, -15.3, -12.2 | -46.9, -44.5, -44.5, -44.5, -21.2 | -5.9 |
| R-OH | -20.2, -15.7, -15.7, -15.7, -15.7 | -26.5, -26.5, -16.6, -10.8, -10.8 | -6.3 |
| R-OP(=O)$(OH)_2$ | -34.2, -34.2, -23.5, -23.5, -23.5 | -44.9, -44.1, -43.7, -43.7, -43.4 | -10.7 |
| R-COOLi | -59.0, -59.0, -48.5, -48.4, -44.8 | -70.2, -70.1, -68.3, -11.9, -11.8 | -11.2 |
| R-$SO_3H$ | -26.5, -26.5, -26.5, -24.5, -22.4 | -42.7, -42.3, -22.3, -12.7, -11.6 | -16.2 |
| R-COOH | -20.8, -12.1, -10.7, -10.4, -10.4 | -37.2, -37.2, -37.2, -8.5, -8.4 | -16.4 |
| R-P(=O)$(OH)_2$ | -26.3, -25.3, -13.6, -12.0, -11.5 | -42.7, -42.7, -27.7, -15.1, -15.1 | -16.4 |

| Functional group | $BE_{SO2}$ | $BE_{H2O}$ | Lowest *BE* of $H_2O$ – Lowest *BE* of $SO_2$ |
|---|---|---|---|
| R-COOCu | -137.1, -137.1, -137.0, -69.4, -14.8 | -97.8, -97.8, -97.8, -10.8, -10.7 | 39.3 |
| R | -14.9, -14.9, -14.8, -14.8, -14.2 | -10.7, -10.6, -6.0, -5.9, -5.3 | 4.2 |
| R-OOH | -20.4, -20.0, -19.1, -14.1, -13.0 | -27.7, -26.5, -26.4, -13.1, -10.7 | -7.3 |
| R-OH | -15.7, -15.3, -12.5, -12.5, -11.8 | -26.5, -26.5, -16.6, -10.8, -10.8 | -10.8 |
| R-P(=O)$(OH)_2$ | -28.6, -28.5, -18.5, -18.4, -16.2 | -42.7, -42.7, -27.7, -15.1, -15.1 | -14.0 |
| R-$HSO_4$ | -31.1, -30.6, -30.6, -30.2, -12.5 | -46.9, -44.5, -44.5, -44.5, -21.2 | -15.8 |
| R-OP(=O)$(OH)_2$ | -28.2, -28.2, -27.5, -25.7, -12.4 | -44.9, -44.1, -43.7, -43.7, -43.4 | -16.7 |
| R-$SO_3H$ | -25.8, -22.6, -20.8, -17.3, -15.1 | -42.7, -42.3, -22.3, -12.7, -11.6 | -16.8 |
| R-COOH | -19.9, -19.9, -14.9, -14.9, -13.2 | -37.2, -37.2, -37.2, -8.5, -8.4 | -17.2 |
| R-COOAg | -32.0, -30.9, -30.7, -28.2, -16.4 | -51.5, -51.5, -51.4, -48.3, -12.3 | -19.5 |
| R-COOLi | -44.9, -42.2, -42.2, -39.0, -15.2 | -70.2, -70.1, -68.3, -11.9, -11.8 | -25.4 |

| Functional group | $BE_{HCN}$ | $BE_{H2O}$ | Lowest *BE* of $H_2O$ – Lowest *BE* of HCN |
|---|---|---|---|
| R-COOCu | -133.4, -126.4, -91.7, -23.3, -14.6 | -97.8, -97.8, -97.8, -10.8, -10.7 | 35.7 |
| R-COOAg | -56.1, -56.1, -56.1, -56.1, -17.0 | -51.5, -51.5, -51.4, -48.3, -12.3 | 4.6 |
| R | -13.9, -13.9, -13.9, -13.9, -13.8 | -10.7, -10.6, -6.0, -5.9, -5.3 | 3.2 |
| R-OH | -21.4, -21.4, -21.4, -15.4, -14.5 | -26.5, -26.5, -16.6, -10.8, -10.8 | -5.1 |
| R-OOH | -21.6, -21.4, -21.4, -15.3, -11.2 | -27.7, -26.5, -26.4, -13.1, -10.7 | -6.1 |
| R-$HSO_4$ | -40.4, -40.4, -18.2, -18.2, -18.1 | -46.9, -44.5, -44.5, -44.5, -21.2 | -6.5 |
| R-OP(=O)$(OH)_2$ | -34.6, -26.4, -25.0, -24.3, -14.1 | -44.9, -44.1, -43.7, -43.7, -43.4 | -10.3 |
| R-COOLi | -59.8, -59.8, -26.6, -26.3, -16.0 | -70.2, -70.1, -68.3, -11.9, -11.8 | -10.5 |
| R-P(=O)$(OH)_2$ | -27.2, -27.2, -25.8, -25.8, -18.8 | -42.7, -42.7, -27.7, -15.1, -15.1 | -15.5 |
| R-$SO_3H$ | -25.9, -25.8, -24.1, -24.1, -20.3 | -42.7, -42.3, -22.3, -12.7, -11.6 | -16.8 |
| R-COOH | -19.7, -19.1, -18.7, -12.0, -11.9 | -37.2, -37.2, -37.2, -8.5, -8.4 | -17.4 |

| Functional group | $BE_{HF}$ | $BE_{H2O}$ | Lowest *BE* of $H_2O$ – Lowest *BE* of HF |
|---|---|---|---|
| R-COOLi | -98.0, -98.0, -97.9, -45.9, -15.5 | -70.2, -70.1, -68.3, -11.9, -11.8 | 27.7 |
| R-P(=O)$(OH)_2$ | -50.5, -50.4, -49.2, -27.1, -24.6 | -42.7, -42.7, -27.7, -15.1, -15.1 | 7.8 |
| R-COOAg | -56.6, -56.4, -56.4, -56.4, -16.2 | -51.5, -51.5, -51.4, -48.3, -12.3 | 5.1 |
| R-COOH | -40.5, -40.5, -32.4, -20.8, -11.0 | -37.2, -37.2, -37.2, -8.5, -8.4 | 3.4 |
| R | -13.9, -13.9, -13.7, -12.8, -3.3 | -10.7, -10.6, -6.0, -5.9, -5.3 | 3.3 |
| R-OP(=O)$(OH)_2$ | -46.6, -46.5, -46.5, -22.3, -20.7 | -44.9, -44.1, -43.7, -43.7, -43.4 | 1.7 |
| R-OH | -28.0, -13.8, -13.8, -13.8, -13.1 | -26.5, -26.5, -16.6, -10.8, -10.8 | 1.5 |
| R-OOH | -26.7, -25.1, -25.1, -21.8, -12.0 | -27.7, -26.5, -26.4, -13.1, -10.7 | -1.0 |
| R-$SO_3H$ | -36.7, -36.2, -36.0, -21.6, -20.5 | -42.7, -42.3, -22.3, -12.7, -11.6 | -6.0 |
| R-$HSO_4$ | -33.9, -33.9, -27.2, -21.5, -21.5 | -46.9, -44.5, -44.5, -44.5, -21.2 | -13.0 |
| R-COOCu | -78.0, -42.0, -42.0, -34.4, -13.6 | -97.8, -97.8, -97.8, -10.8, -10.7 | -19.8 |

| Functional group | $BE_{CH3Br}$ | $BE_{H2O}$ | Lowest *BE* of $H_2O$ – Lowest *BE* of $CH_3Br$ |
|---|---|---|---|
| R-COOAg | -75.0, -75.0, -70.5, -42.2, -41.5 | -51.5, -51.5, -51.4, -48.3, -12.3 | 23.5 |
| R | -10.6, -4.3, -2.8, -2.7, -2.7 | -10.7, -10.6, -6.0, -5.9, -5.3 | -0.1 |
| R-COOCu | -91.4, -90.9, -81.4, -11.2, -9.9 | -97.8, -97.8, -97.8, -10.8, -10.7 | -6.4 |
| R-OOH | -15.4, -15.4, -10.2, -10.0, -9.9 | -27.7, -26.5, -26.4, -13.1, -10.7 | -12.3 |
| R-OH | -10.8, -10.8, -10.5, -9.1, -6.6 | -26.5, -26.5, -16.6, -10.8, -10.8 | -15.7 |
| R-$HSO_4$ | -29.3, -27.8, -27.8, -27.3, -6.0 | -46.9, -44.5, -44.5, -44.5, -21.2 | -17.6 |
| R-COOH | -19.1, -9.2, -6.6, -6.5, -5.8 | -37.2, -37.2, -37.2, -8.5, -8.4 | -18.1 |
| R-OP(=O)$(OH)_2$ | -25.0, -25.0, -24.2, -24.2, -11.9 | -44.9, -44.1, -43.7, -43.7, -43.4 | -19.9 |
| R-$SO_3H$ | -22.2, -22.2, -19.9, -19.8, -7.6 | -42.7, -42.3, -22.3, -12.7, -11.6 | -20.5 |
| R-P(=O)$(OH)_2$ | -22.0, -21.8, -11.0, -7.5, -7.4 | -42.7, -42.7, -27.7, -15.1, -15.1 | -20.7 |
| R-COOLi | -43.8, -43.7, -38.8, -12.2, 112.9 | -70.2, -70.1, -68.3, -11.9, -11.8 | -26.5 |

| Functional group | $BE_{H2S}$ | $BE_{H2O}$ | Lowest *BE* of $H_2O$ – Lowest *BE* of $H_2S$ |
|---|---|---|---|
| R-COOCu | -115.7, -115.7, -112.6, -12.3, -9.5 | -97.8, -97.8, -97.8, -10.8, -10.7 | 18.0 |
| R | -10.9, -10.9, -10.9, -10.9, -7.8 | -10.7, -10.6, -6.0, -5.9, -5.3 | 0.3 |
| R-COOAg | -51.3, -51.3, -51.3, -14.9, -10.9 | -51.5, -51.5, -51.4, -48.3, -12.3 | -0.2 |
| R-OH | -12.7, -12.7, -12.4, -11.3, -6.9 | -26.5, -26.5, -16.6, -10.8, -10.8 | -13.8 |
| R-OOH | -11.6, -11.5, -11.0, -10.2, -9.0 | -27.7, -26.5, -26.4, -13.1, -10.7 | -16.2 |
| R-$HSO_4$ | -29.8, -29.8, -29.8, -27.0, -5.7 | -46.9, -44.5, -44.5, -44.5, -21.2 | -17.1 |
| R-$OP(=O)(OH)_2$ | -25.8, -22.4, -21.8, -21.6, -17.6 | -44.9, -44.1, -43.7, -43.7, -43.4 | -19.1 |
| R-COOH | -15.8, -10.1, -9.8, -9.4, -6.1 | -37.2, -37.2, -37.2, -8.5, -8.4 | -21.4 |
| R-$P(=O)(OH)_2$ | -20.7, -19.5, -19.5, -12.3, -10.1 | -42.7, -42.7, -27.7, -15.1, -15.1 | -22.0 |
| R-$SO_3H$ | -20.6, -19.8, -19.8, -18.5, -14.9 | -42.7, -42.3, -22.3, -12.7, -11.6 | -22.1 |
| R-COOLi | -37.9, -37.2, -37.1, -13.6, -12.0 | -70.2, -70.1, -68.3, -11.9, -11.8 | -32.3 |

| Functional group | $BE_{HNO3}$ | $BE_{H2O}$ | Lowest *BE* of $H_2O$ – Lowest *BE* of $HNO_3$ |
|---|---|---|---|
| R-$P(=O)(OH)_2$ | -58.2, -56.9, -29.7, -23.7, -11.0 | -42.7, -42.7, -27.7, -15.1, -15.1 | 15.6 |
| R-COOLi | -85.8, -45.8, -38.6, -36.3, -15.0 | -70.2, -70.1, -68.3, -11.9, -11.8 | 15.5 |
| R | -17.9, -17.9, -16.8, -14.3, -13.9 | -10.7, -10.6, -6.0, -5.9, -5.3 | 7.3 |
| R-$OP(=O)(OH)_2$ | -51.3, -51.3, -28.9, -25.1, -22.5 | -44.9, -44.1, -43.7, -43.7, -43.4 | 6.4 |
| R-OOH | -32.2, -27.4, -23.0, -19.3, -13.6 | -27.7, -26.5, -26.4, -13.1, -10.7 | 4.5 |
| R-$SO_3H$ | -43.9, -29.1, -29.1, -26.7, -23.8 | -42.7, -42.3, -22.3, -12.7, -11.6 | 1.3 |
| R-$HSO_4$ | -46.2, -46.2, -27.0, -27.0, -23.7 | -46.9, -44.5, -44.5, -44.5, -21.2 | -0.7 |
| R-COOAg | -48.6, -39.2, -39.0, -26.8, -2.1 | -51.5, -51.5, -51.4, -48.3, -12.3 | -2.9 |
| R-COOH | -33.5, -32.7, -32.0, -19.4, -17.3 | -37.2, -37.2, -37.2, -8.5, -8.4 | -3.7 |
| R-OH | -17.6, -17.5, -15.3, 65.0, 336.1 | -26.5, -26.5, -16.6, -10.8, -10.8 | -9.0 |
| R-COOCu | -63.4, -59.2, -43.2, -41.3, -41.1 | -97.8, -97.8, -97.8, -10.8, -10.7 | -34.4 |

| Functional group | $BE_{HCHO}$ | $BE_{H2O}$ | Lowest *BE* of $H_2O$ – Lowest *BE* of HCHO |
|---|---|---|---|
| R-COOCu | -101.7, -101.7, -101.7, -101.3, -9.0 | -97.8, -97.8, -97.8, -10.8, -10.7 | 3.9 |
| R | -12.2, -12.1, -12.1, -11.1, -10.9 | -10.7, -10.6, -6.0, -5.9, -5.3 | 1.5 |
| R-COOAg | -50.8, -50.8, -50.8, -50.6, -9.4 | -51.5, -51.5, -51.4, -48.3, -12.3 | -0.7 |
| R-OOH | -26.4, -25.9, -25.9, -11.8, -10.3 | -27.7, -26.5, -26.4, -13.1, -10.7 | -1.3 |
| R-COOLi | -68.0, -68.0, -68.0, -68.0, -9.2 | -70.2, -70.1, -68.3, -11.9, -11.8 | -2.3 |
| R-OH | -23.6, -23.6, -23.5, -12.3, -10.6 | -26.5, -26.5, -16.6, -10.8, -10.8 | -2.9 |
| R-P(=O)$(OH)_2$ | -38.9, -38.9, -36.8, -12.9, -11.4 | -42.7, -42.7, -27.7, -15.1, -15.1 | -3.8 |
| R-OP(=O)$(OH)_2$ | -40.5, -39.1, -39.1, -35.7, -12.3 | -44.9, -44.1, -43.7, -43.7, -43.4 | -4.4 |
| R-COOH | -32.2, -12.5, -12.5, -10.7, -9.4 | -37.2, -37.2, -37.2, -8.5, -8.4 | -4.9 |
| R-$SO_3H$ | -37.4, -37.4, -37.2, -17.3, -10.2 | -42.7, -42.3, -22.3, -12.7, -11.6 | -5.3 |
| R-$HSO_4$ | -38.1, -38.1, -38.1, -16.4, -9.0 | -46.9, -44.5, -44.5, -44.5, -21.2 | -8.8 |

| Functional group | $BE_{COCl2}$ | $BE_{H2O}$ | Lowest *BE* of $H_2O$ – Lowest *BE* of $COCl_2$ |
|---|---|---|---|
| R | -12.6, -12.2, -12.2, -12.1, 0.0 | -10.7, -10.6, -6.0, -5.9, -5.3 | 2.0 |
| R-OOH | -20.4, -15.1, -13.3, -11.7, -9.8 | -27.7, -26.5, -26.4, -13.1, -10.7 | -7.4 |
| R-OH | -14.6, -13.1, -13.1, -11.8, -5.3 | -26.5, -26.5, -16.6, -10.8, -10.8 | -12.0 |
| R-$HSO_4$ | -30.4, -30.4, -26.8, -15.2, -8.4 | -46.9, -44.5, -44.5, -44.5, -21.2 | -16.5 |
| R-OP(=O)$(OH)_2$ | -25.6, -24.8, -16.8, -16.8, -5.6 | -44.9, -44.1, -43.7, -43.7, -43.4 | -19.4 |
| R-COOH | -16.7, -12.8, -12.7, -12.7, -6.3 | -37.2, -37.2, -37.2, -8.5, -8.4 | -20.5 |
| R-$SO_3H$ | -21.9, -21.8, -19.7, -14.6, -12.1 | -42.7, -42.3, -22.3, -12.7, -11.6 | -20.8 |
| R-P(=O)$(OH)_2$ | -19.3, -19.3, -18.6, -17.8, -14.9 | -42.7, -42.7, -27.7, -15.1, -15.1 | -23.3 |
| R-COOAg | -25.7, -25.7, -23.8, -13.1, -9.8 | -51.5, -51.5, -51.4, -48.3, -12.3 | -25.8 |
| R-COOCu | -70.5, -70.4, -69.9, -13.1, -7.7 | -97.8, -97.8, -97.8, -10.8, -10.7 | -27.3 |
| R-COOLi | -38.6, -36.3, -36.3, -13.4, -8.2 | -70.2, -70.1, -68.3, -11.9, -11.8 | -31.6 |

| Functional group | $BE_{CO2}$ | $BE_{H2O}$ | Lowest *BE* of $H_2O$ – Lowest *BE* of $CO_2$ |
|---|---|---|---|
| R | -8.9, -8.9, -8.9, -1.8, -1.8 | -10.7, -10.6, -6.0, -5.9, -5.3 | -1.7 |
| R-OOH | -13.1, -11.7, -11.7, -11.2, -9.2 | -27.7, -26.5, -26.4, -13.1, -10.7 | -14.7 |
| R-OH | -10.3, -9.5, -9.4, -9.3, -8.3 | -26.5, -26.5, -16.6, -10.8, -10.8 | -16.3 |
| R-COOH | -13.8, -13.8, -13.8, -8.2, -7.6 | -37.2, -37.2, -37.2, -8.5, -8.4 | -23.4 |
| R-$HSO_4$ | -21.1, -21.1, -21.1, -21.1, -8.0 | -46.9, -44.5, -44.5, -44.5, -21.2 | -25.8 |
| R-$OP(=O)(OH)_2$ | -19.0, -19.0, -17.7, -17.7, -13.4 | -44.9, -44.1, -43.7, -43.7, -43.4 | -25.9 |
| R-$P(=O)(OH)_2$ | -16.7, -15.5, -15.5, -12.5, -10.8 | -42.7, -42.7, -27.7, -15.1, -15.1 | -26.0 |
| R-$SO_3H$ | -15.2, -15.0, -14.2, -10.4, -10.0 | -42.7, -42.3, -22.3, -12.7, -11.6 | -27.5 |
| R-COOAg | -17.7, -16.1, -14.4, -14.3, -9.2 | -51.5, -51.5, -51.4, -48.3, -12.3 | -33.8 |
| R-COOLi | -30.5, -30.5, -30.5, -27.7, -8.9 | -70.2, -70.1, -68.3, -11.9, -11.8 | -39.7 |
| R-COOCu | -40.1, -39.7, -39.7, -39.7, -8.8 | -97.8, -97.8, -97.8, -10.8, -10.7 | -57.7 |

| Functional group | $BE_{Cl2}$ | $BE_{H2O}$ | Lowest *BE* of $H_2O$ – Lowest *BE* of $Cl_2$ |
|---|---|---|---|
| R | -8.2, -4.4, -1.7, -1.7, -1.6 | -10.7, -10.6, -6.0, -5.9, -5.3 | -2.4 |
| R-OH | -9.0, -5.2, -4.8, -2.9, 0.1 | -26.5, -26.5, -16.6, -10.8, -10.8 | -17.5 |
| R-OOH | -8.2, -8.2, -8.1, -5.2, -5.2 | -27.7, -26.5, -26.4, -13.1, -10.7 | -19.5 |
| R-COOH | -7.6, -5.7, -5.7, -2.4, -0.7 | -37.2, -37.2, -37.2, -8.5, -8.4 | -29.6 |
| R-$P(=O)(OH)_2$ | -10.8, -7.3, -7.2, -7.0, -0.9 | -42.7, -42.7, -27.7, -15.1, -15.1 | -31.9 |
| R-$OP(=O)(OH)_2$ | -10.1, -8.0, -7.6, -7.5, -4.9 | -44.9, -44.1, -43.7, -43.7, -43.4 | -34.8 |
| R-$SO_3H$ | -7.3, -6.6, -3.5, 0.4, 0.5 | -42.7, -42.3, -22.3, -12.7, -11.6 | -35.4 |
| R-$HSO_4$ | -11.3, -10.7, -8.8, -6.0, -5.9 | -46.9, -44.5, -44.5, -44.5, -21.2 | -35.6 |
| R-COOAg | -12.4, -9.9, -9.7, -9.0, -0.3 | -51.5, -51.5, -51.4, -48.3, -12.3 | -39.1 |
| R-COOCu | -54.8, -54.8, -54.8, -54.8, -9.0 | -97.8, -97.8, -97.8, -10.8, -10.7 | -43.0 |
| R-COOLi | -15.2, -9.5, -5.5, -5.4, -5.3 | -70.2, -70.1, -68.3, -11.9, -11.8 | -55.0 |

**Table S2**: Calculated free energies of adsorption at 298 K in kJ/mol of toxic industrial chemicals ($\Delta G_{TIC}$) and water ($\Delta G_{H2O}$) binding with ten functional group candidates. The last column represents the difference between the adsorption free energy of water and the adsorption free energy of the toxic industrial chemical for each case. A positive value indicates that the binding of the toxic industrial chemical is more stable than that of water.

| **Functional group** | $\Delta G_{H2SO4}$ | $\Delta G_{H2O}$ | $\Delta G$ $H_2O$ – $\Delta G$ $H_2SO_4$ |
|---|---|---|---|
| R-COOCu | -124.8 | -52.0 | 72.8 |
| R-P(=O)$(OH)_2$ | -27.9 | 5.2 | 33.1 |
| R-COOAg | -41.2 | -8.8 | 32.4 |
| R-COOLi | -62.2 | -30.8 | 31.4 |
| R-OP(=O)$(OH)_2$ | -15.6 | 1.9 | 17.6 |
| R-COOH | -7.7 | 9.1 | 16.8 |
| R-OH | 3.1 | 12.4 | 9.4 |
| R-$SO_3$H | -0.3 | 6.7 | 6.9 |
| R-OOH | 10.0 | 15.7 | 5.6 |
| R | 15.7 | 20.4 | 4.6 |
| R-$HSO_4$ | -6.3 | -1.8 | 4.5 |

| **Functional group** | $\Delta G_{CO}$ | $\Delta G_{H2O}$ | $\Delta G$ $H_2O$ – $\Delta G$ CO |
|---|---|---|---|
| R-COOCu | -120.1 | -52.0 | 68.1 |
| R-COOAg | -5.1 | -8.8 | -3.7 |
| R | 24.1 | 20.4 | -3.7 |
| R-OH | 20.8 | 12.4 | -8.3 |
| R-$SO_3$H | 15.2 | 6.7 | -8.5 |
| R-OOH | 25.0 | 15.7 | -9.3 |
| R-COOH | 22.6 | 9.1 | -13.5 |
| R-P(=O)$(OH)_2$ | 22.6 | 5.2 | -17.4 |
| R-OP(=O)$(OH)_2$ | 21.4 | 1.9 | -19.5 |
| R-$HSO_4$ | 21.1 | -1.8 | -22.9 |
| R-COOLi | 4.3 | -30.8 | -35.1 |

| Functional group | $\Delta G_{HCl}$ | $\Delta G_{H2O}$ | $\Delta G$ $H_2O$ – $\Delta G$ HCl |
|---|---|---|---|
| R-COOCu | -111.9 | -52.0 | 59.9 |
| R-COOAg | -36.1 | -8.8 | 27.3 |
| R-COOLi | -35.9 | -30.8 | 5.1 |
| R | 20.5 | 20.4 | -0.2 |
| R-OOH | 18.3 | 15.7 | -2.6 |
| R-OH | 20.1 | 12.4 | -7.6 |
| R-P(=O)$(OH)_2$ | 13.5 | 5.2 | -8.3 |
| R-COOH | 19.0 | 9.1 | -9.9 |
| R-OP(=O)$(OH)_2$ | 15.4 | 1.9 | -13.5 |
| R-$SO_3$H | 20.7 | 6.7 | -14.0 |
| R-$HSO_4$ | 23.3 | -1.8 | -25.1 |

| Functional group | $\Delta G_{CNCl}$ | $\Delta G_{H2O}$ | $\Delta G$ $H_2O$ – $\Delta G$ CNCl |
|---|---|---|---|
| R-COOCu | -88.8 | -52.0 | 36.8 |
| R-COOAg | -18.6 | -8.8 | 9.8 |
| R-OH | 12.5 | 12.4 | 0.0 |
| R-OOH | 18.1 | 15.7 | -2.4 |
| R | 23.3 | 20.4 | -3.0 |
| R-COOH | 12.7 | 9.1 | -3.6 |
| R-$HSO_4$ | 3.2 | -1.8 | -5.0 |
| R-COOLi | -23.0 | -30.8 | -7.8 |
| R-$SO_3$H | 15.1 | 6.7 | -8.4 |
| R-P(=O)$(OH)_2$ | 14.1 | 5.2 | -8.9 |
| R-OP(=O)$(OH)_2$ | 11.7 | 1.9 | -9.8 |

| Functional group | $\Delta G_{SO2}$ | $\Delta G_{H2O}$ | $\Delta G$ $H_2O$ – $\Delta G$ $SO_2$ |
|---|---|---|---|
| R-COOCu | -78.5 | -52.0 | 26.5 |
| R | 24.4 | 20.4 | -4.1 |
| R-OOH | 26.4 | 15.7 | -10.8 |
| R-OH | 24.5 | 12.4 | -12.0 |
| R-COOH | 21.3 | 9.1 | -12.2 |
| R-$SO_3$H | 23.0 | 6.7 | -16.4 |
| R-P(=O)$(OH)_2$ | 23.1 | 5.2 | -17.9 |
| R-$HSO_4$ | 17.9 | -1.8 | -19.7 |
| R-OP(=O)$(OH)_2$ | 22.8 | 1.9 | -20.9 |
| R-COOAg | 14.9 | -8.8 | -23.7 |
| R-COOLi | 1.2 | -30.8 | -32.1 |

| Functional group | $\Delta G_{HCN}$ | $\Delta G_{H2O}$ | $\Delta G$ $H_2O$ – $\Delta G$ HCN |
|---|---|---|---|
| R-COOCu | -87.7 | -52.0 | 35.7 |
| R-COOAg | -19.2 | -8.8 | 10.4 |
| R | 17.5 | 20.4 | 2.9 |
| R-OH | 10.7 | 12.4 | 1.7 |
| R-OOH | 18.0 | 15.7 | -2.3 |
| R-$SO_3H$ | 9.7 | 6.7 | -3.0 |
| R-COOH | 12.7 | 9.1 | -3.6 |
| R-$HSO_4$ | 4.6 | -1.8 | -6.4 |
| R-P(=O)$(OH)_2$ | 12.8 | 5.2 | -7.6 |
| R-COOLi | -22.8 | -30.8 | -8.0 |
| R-OP(=O)$(OH)_2$ | 11.4 | 1.9 | -9.5 |

| Functional group | $\Delta G_{HF}$ | $\Delta G_{H2O}$ | $\Delta G$ $H_2O$ – $\Delta G$ HF |
|---|---|---|---|
| R-COOLi | -51.8 | -30.8 | 21.0 |
| R-P(=O)$(OH)_2$ | -5.9 | 5.2 | 11.1 |
| R-COOAg | -17.2 | -8.8 | 8.4 |
| R-COOH | 4.0 | 9.1 | 5.1 |
| R-OP(=O)$(OH)_2$ | -1.0 | 1.9 | 3.0 |
| R-OH | 9.6 | 12.4 | 2.9 |
| R-OOH | 13.6 | 15.7 | 2.1 |
| R | 18.8 | 20.4 | 1.6 |
| R-$SO_3H$ | 7.7 | 6.7 | -1.1 |
| R-$HSO_4$ | 11.2 | -1.8 | -13.0 |
| R-COOCu | -31.6 | -52.0 | -20.4 |

| Functional group | $\Delta G_{CH3Br}$ | $\Delta G_{H2O}$ | $\Delta G$ $H_2O$ – $\Delta G$ $CH_3Br$ |
|---|---|---|---|
| R-COOAg | -34.3 | -8.8 | 25.5 |
| R-COOCu | -47.3 | -52.0 | -4.7 |
| R | 28.2 | 20.4 | -7.9 |
| R-$SO_3H$ | 16.0 | 6.7 | -9.4 |
| R-COOH | 20.6 | 9.1 | -11.5 |
| R-OOH | 27.6 | 15.7 | -12.0 |
| R-OH | 29.6 | 12.4 | -17.2 |
| R-P(=O)$(OH)_2$ | 23.2 | 5.2 | -18.0 |
| R-$HSO_4$ | 19.7 | -1.8 | -21.5 |
| R-OP(=O)$(OH)_2$ | 28.0 | 1.9 | -26.1 |
| R-COOLi | -2.5 | -30.8 | -28.3 |

| Functional group | $\Delta G_{H2S}$ | $\Delta G_{H2O}$ | $\Delta G$ $H_2O$ – $\Delta G$ $H_2S$ |
|---|---|---|---|
| R-COOCu | -70.0 | -52.0 | 17.9 |
| R-COOAg | -12.3 | -8.8 | 3.5 |
| R | 24.5 | 20.4 | -4.1 |
| R-OH | 21.6 | 12.4 | -9.2 |
| R-COOH | 22.2 | 9.1 | -13.1 |
| R-OOH | 30.2 | 15.7 | -14.5 |
| R-$SO_3H$ | 22.6 | 6.7 | -16.0 |
| R-P(=O)$(OH)_2$ | 21.6 | 5.2 | -16.5 |
| R-$HSO_4$ | 17.8 | -1.8 | -19.6 |
| R-OP(=O)$(OH)_2$ | 22.5 | 1.9 | -20.6 |
| R-COOLi | 2.6 | -30.8 | -33.5 |

| Functional group | $\Delta G_{HNO3}$ | $\Delta G_{H2O}$ | $\Delta G$ $H_2O$ – $\Delta G$ $HNO_3$ |
|---|---|---|---|
| R-P(=O)$(OH)_2$ | -7.7 | 5.2 | 12.9 |
| R-COOLi | -35.6 | -30.8 | 4.8 |
| R-OP(=O)$(OH)_2$ | 0.8 | 1.9 | 1.1 |
| R-OOH | 16.2 | 15.7 | -0.6 |
| R-$SO_3H$ | 7.6 | 6.7 | -0.9 |
| R | 21.4 | 20.4 | -1.0 |
| R-COOH | 11.9 | 9.1 | -2.8 |
| R-COOAg | -2.8 | -8.8 | -6.0 |
| R-$HSO_4$ | 11.0 | -1.8 | -12.8 |
| R-OH | 27.4 | 12.4 | -15.0 |
| R-COOCu | -15.7 | -52.0 | -36.3 |

| Functional group | $\Delta G_{HCHO}$ | $\Delta G_{H2O}$ | $\Delta G$ $H_2O$ – $\Delta G$ HCHO |
|---|---|---|---|
| R-COOCu | -49.3 | -52.0 | -2.7 |
| R-$SO_3H$ | 9.6 | 6.7 | -2.9 |
| R-COOH | 12.8 | 9.1 | -3.7 |
| R-COOAg | -4.7 | -8.8 | -4.1 |
| R-P(=O)$(OH)_2$ | 10.5 | 5.2 | -5.3 |
| R-OOH | 21.5 | 15.7 | -5.9 |
| R | 26.5 | 20.4 | -6.2 |
| R-OH | 18.6 | 12.4 | -6.2 |
| R-COOLi | -22.1 | -30.8 | -8.7 |
| R-OP(=O)$(OH)_2$ | 14.1 | 1.9 | -12.2 |
| R-$HSO_4$ | 11.9 | -1.8 | -13.7 |

| Functional group | $\Delta G_{COCl2}$ | $\Delta G_{H2O}$ | $\Delta G$ $H_2O$ – $\Delta G$ $COCl_2$ |
|---|---|---|---|
| R | 31.3 | 20.4 | -10.9 |
| R-OOH | 32.5 | 15.7 | -16.9 |
| R-COOH | 26.1 | 9.1 | -17.0 |
| R-OH | 30.4 | 12.4 | -18.0 |
| R-$SO_3H$ | 26.1 | 6.7 | -19.4 |
| R-COOAg | 13.5 | -.8.8 | -22.3 |
| R-$HSO_4$ | 22.7 | -1.8 | -24.5 |
| R-$P(=O)(OH)_2$ | 30.3 | 5.2 | -25.1 |
| R-$OP(=O)(OH)_2$ | 30.3 | 1.9 | -28.4 |
| R-COOCu | -21.2 | -52.0 | -30.8 |
| R-COOLi | 5.7 | -30.8 | -36.6 |

| Functional group | $\Delta G_{CO2}$ | $\Delta G_{H2O}$ | $\Delta G$ $H_2O$ – $\Delta G$ $CO_2$ |
|---|---|---|---|
| R | 18.7 | 20.4 | 1.6 |
| R-OH | 18.7 | 12.4 | -6.3 |
| R-OOH | 23.3 | 15.7 | -7.6 |
| R-COOH | 20.3 | 9.1 | -11.2 |
| R-$P(=O)(OH)_2$ | 19.9 | 5.2 | -14.8 |
| R-$SO_3H$ | 21.6 | 6.7 | -14.9 |
| R-$HSO_4$ | 19.0 | -1.8 | -20.8 |
| R-$OP(=O)(OH)_2$ | 22.7 | 1.9 | -20.8 |
| R-COOAg | 15.1 | -8.8 | -23.9 |
| R-COOLi | 5.1 | -30.8 | -35.9 |
| R-COOCu | -4.3 | -52.0 | -47.7 |

| Functional group | $\Delta G_{Cl2}$ | $\Delta G_{H2O}$ | $\Delta G$ $H_2O$ – $\Delta G$ $Cl_2$ |
|---|---|---|---|
| R | 25.6 | 20.4 | -5.2 |
| R-OOH | 27.2 | 15.7 | -11.5 |
| R-OH | 25.7 | 12.4 | -13.3 |
| R-$SO_3H$ | 24.5 | 6.7 | -17.9 |
| R-COOH | 29.1 | 9.1 | -20.0 |
| R-$P(=O)(OH)_2$ | 25.8 | 5.2 | -20.6 |
| R-$HSO_4$ | 25.3 | -1.8 | -27.1 |
| R-$OP(=O)(OH)_2$ | 30.2 | 1.9 | -28.3 |
| R-COOAg | 24.3 | -8.8 | -33.1 |
| R-COOCu | -13.1 | -52.0 | -38.9 |
| R-COOLi | 21.3 | -30.8 | -52.2 |

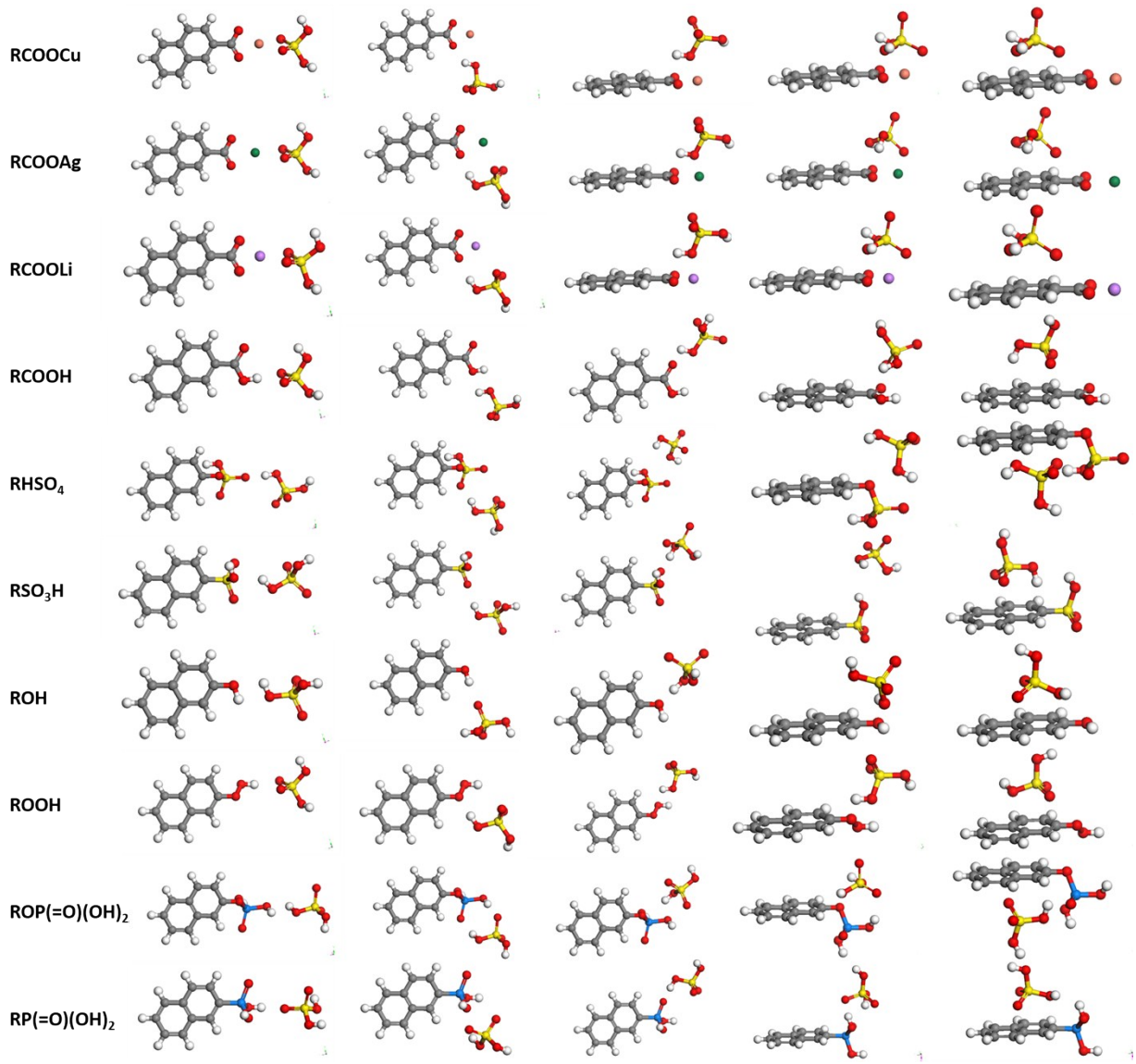


**Figure S1.** Five different initial positions for $H_2SO_4$ binding to each of the ten functional groups. Atoms in grey, white, red, brown, yellow, dark green, violet, and cyan, represent carbon, hydrogen, oxygen, copper, sulfur, silver, lithium, and phosphorus, respectively.

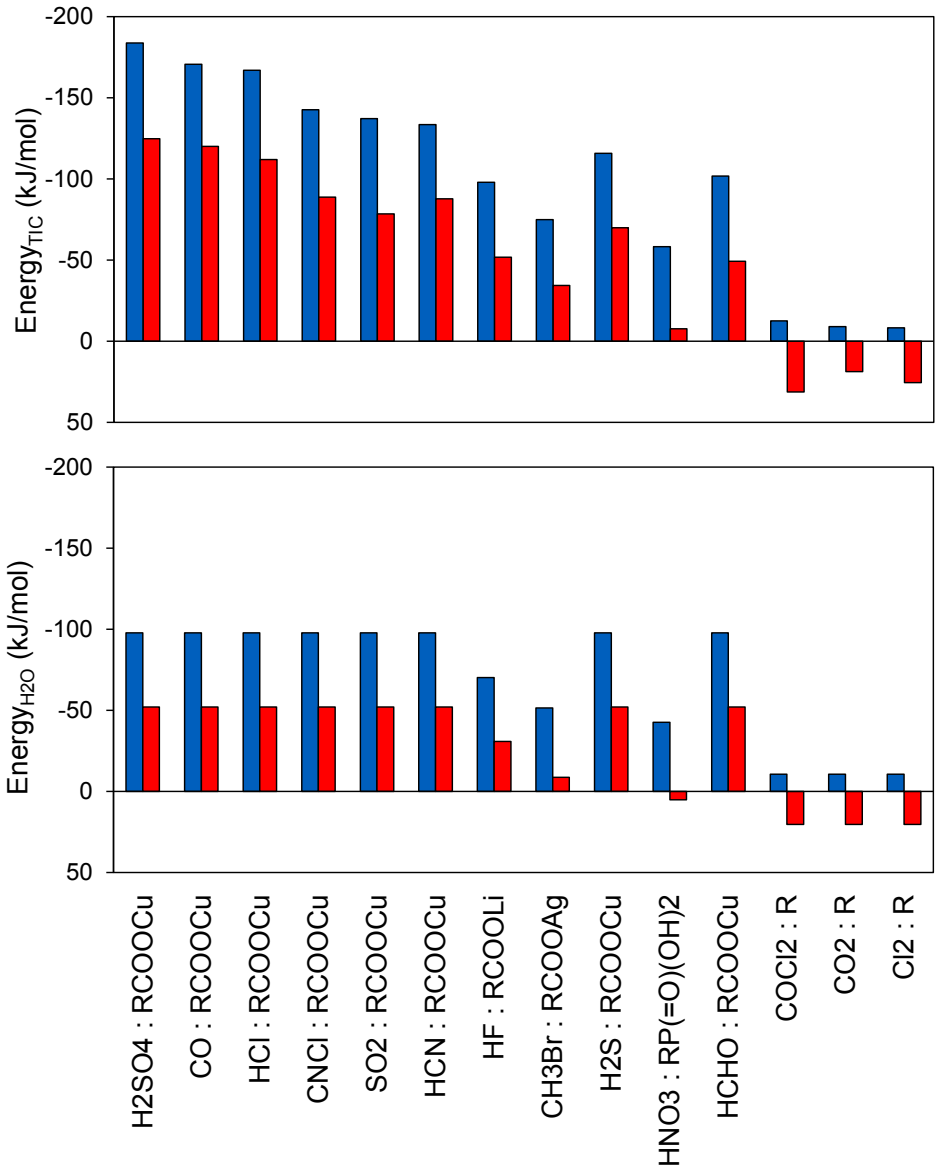


**Figure S2.** Comparison between *BE* (*blue bars*) and Δ*G* (*red bars*) listed in Table 2 for the TICs (*top*) and water (*bottom*).

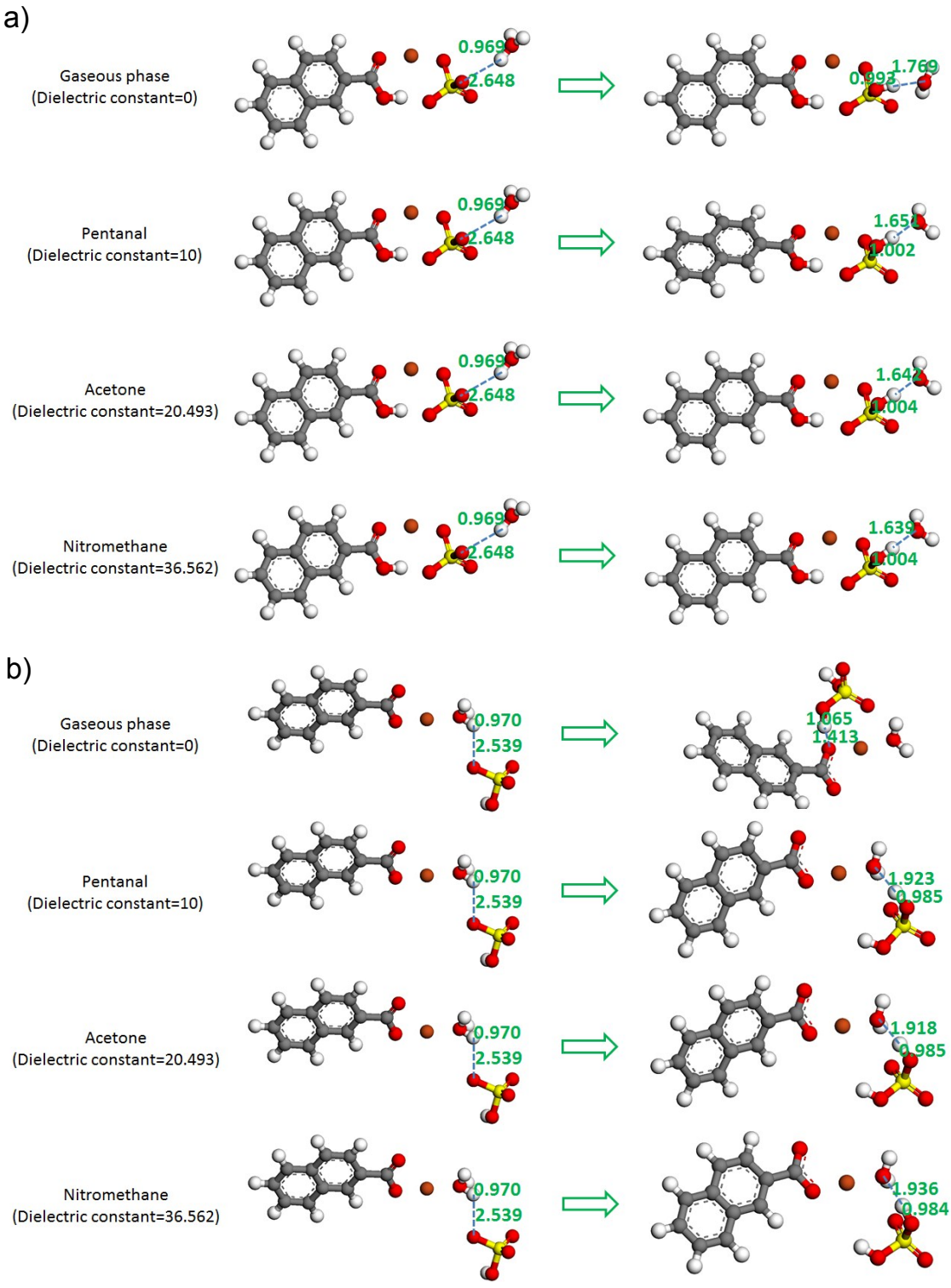


**Figure S3:** Initial (*left*) and optimized (*right*) clusters associated with **a)** $H_3O^+$ on RCOOCu_$HSO_4^-$ and **b)** $HSO_4^-$ on RCOOCu_$H_3O^+$ using different dielectric constants. Atoms in grey, white, red, blue, yellow and brown represent carbon, hydrogen, oxygen, nitrogen, sulfur and copper, respectively. Values in green represent binding distances in Å