Mechanistic Insights from Discrete Molecular Dynamics Simulations of Pesticide–Nanoparticle Interactions, Supplementary Information

Nicholas K Geitner,[a] Weilu Zhao,[b] Feng Ding,[c] Wei Chen,[b] Mark R Wiesner[a*]

Summary:

Seven figures and 1 table on 5 pages

Table S1. Summary of fiber–water distribution coefficients (K_{fiber}) of the adsorbates.

Adsorbate	log K_{fiber} [a]	R^2	N [b]
Tefluthrin	6.44±0.25	0.988	5
Chlorpyrifos	5.25±0.02	0.997	7
p'p-DDE	7.07±0.11	0.994	6
cis-Chlordane	6.79±0.22	0.991	5
trans-Chlordane	6.51±0.13	0.996	5
Bifenthrin	7.22±0.11	0.997	5
cis-Permethrin	4.35±0.39	0.943	4
trans-Permethrin	4.45±0.20	0.985	4

[a] K_{fiber} values were obtained by fitting the fiber sorption isotherms with the linear sorption model, i.e., $C_{fiber} = K_{fiber} \cdot C_W$; values after ± sign indicate relative standard deviation.

[b] Number of data points in fiber sorption isotherm.

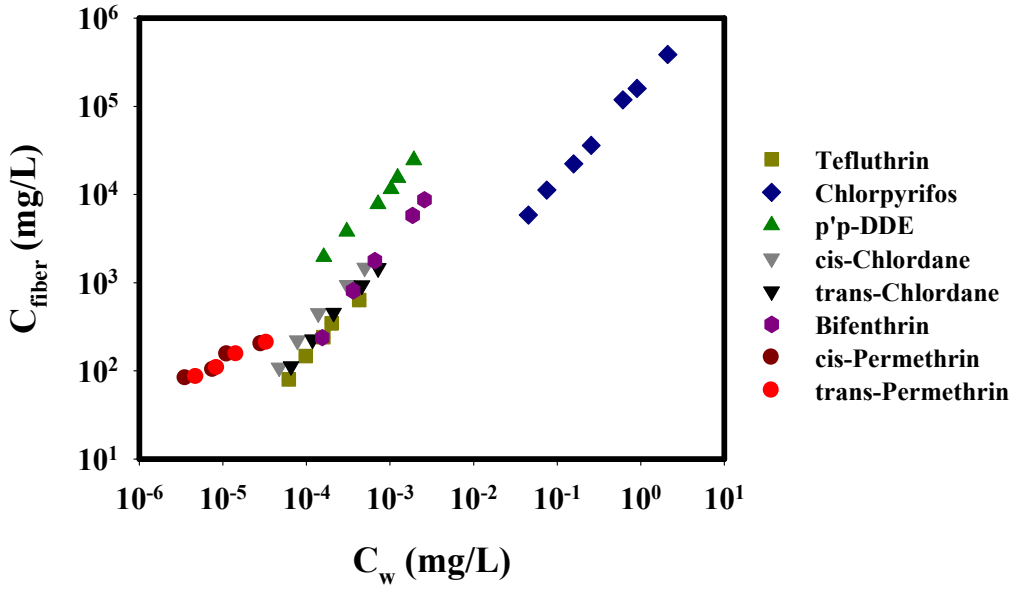

Figure. S1. Sorption isotherms of different adsorbates to polyacrylate fibers.

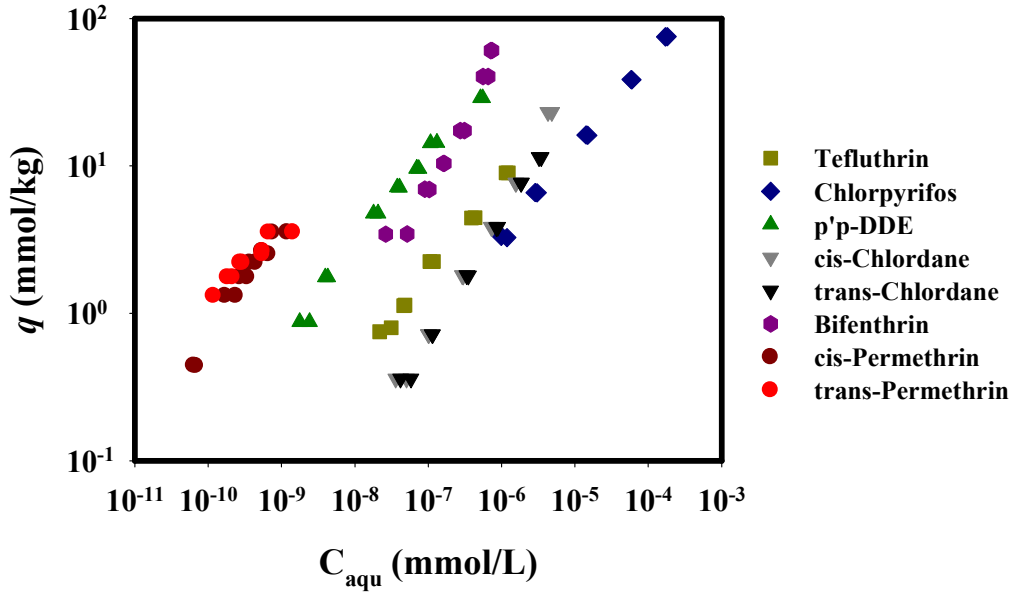

Figure. S2. Sorption isotherms of different adsorbates to nC_{60}.

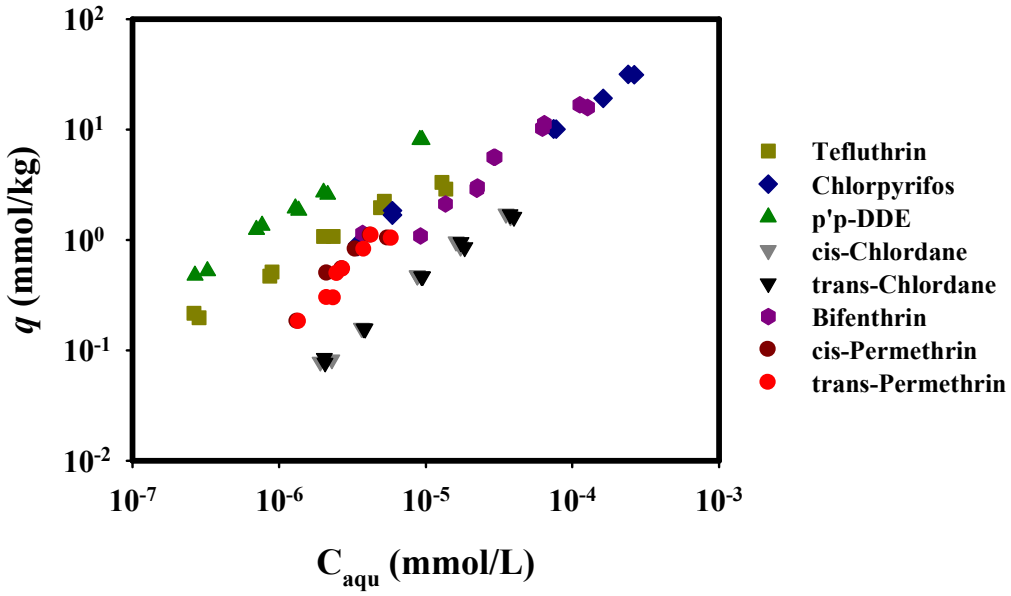

Figure. S3. Sorption isotherms of different adsorbates to $nCeO_2$.

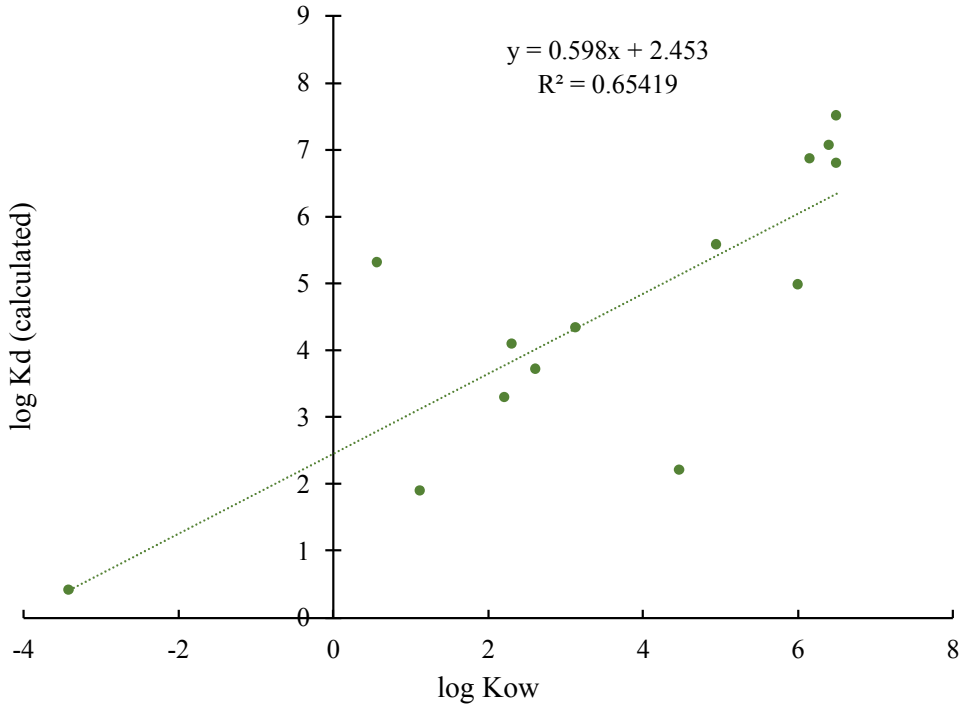

Figure S4. Correlation between K_{ow} and DMD simulated K_d values for Fullerenes

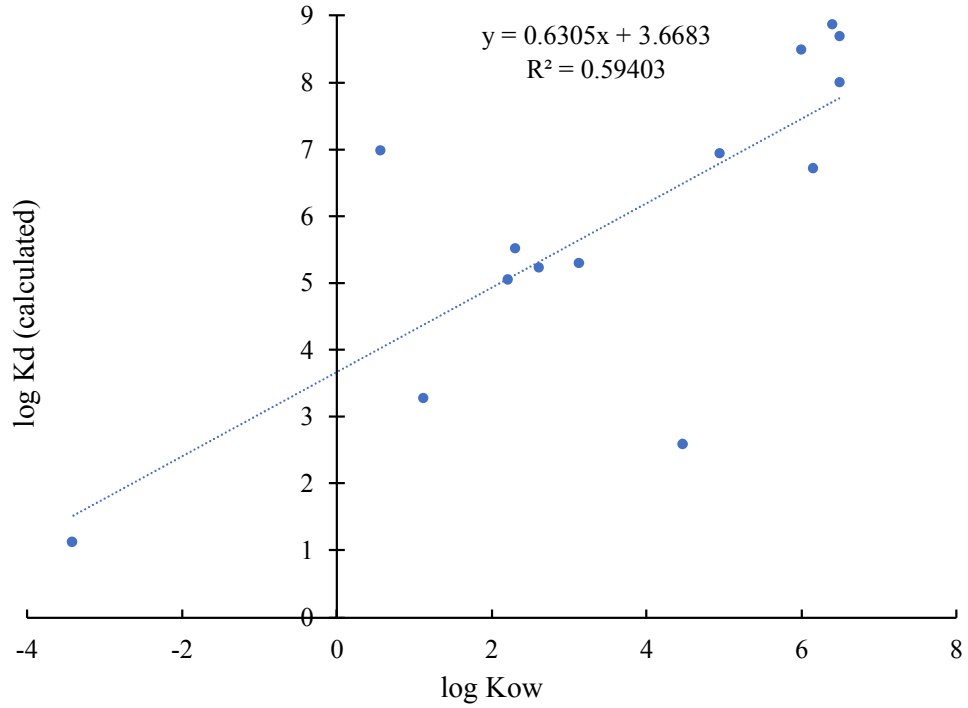

Figure S5. Correlation between K_{ow} and DMD simulated K_d values for Fullerol-8

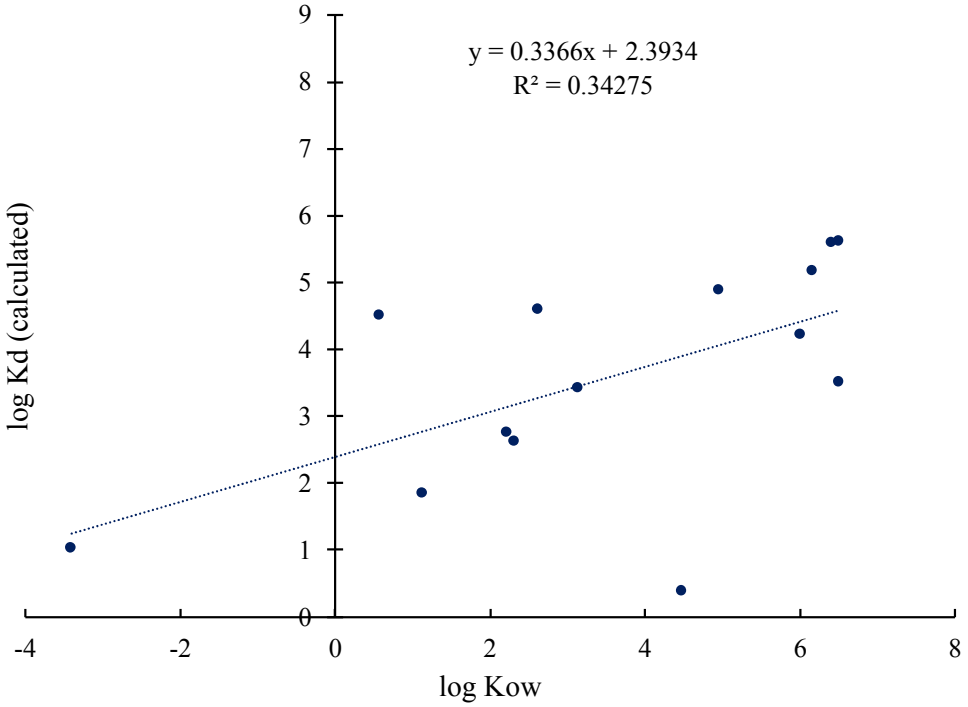

Figure S6. Correlation between K_{ow} and DMD simulated K_d values for Fullerol-24

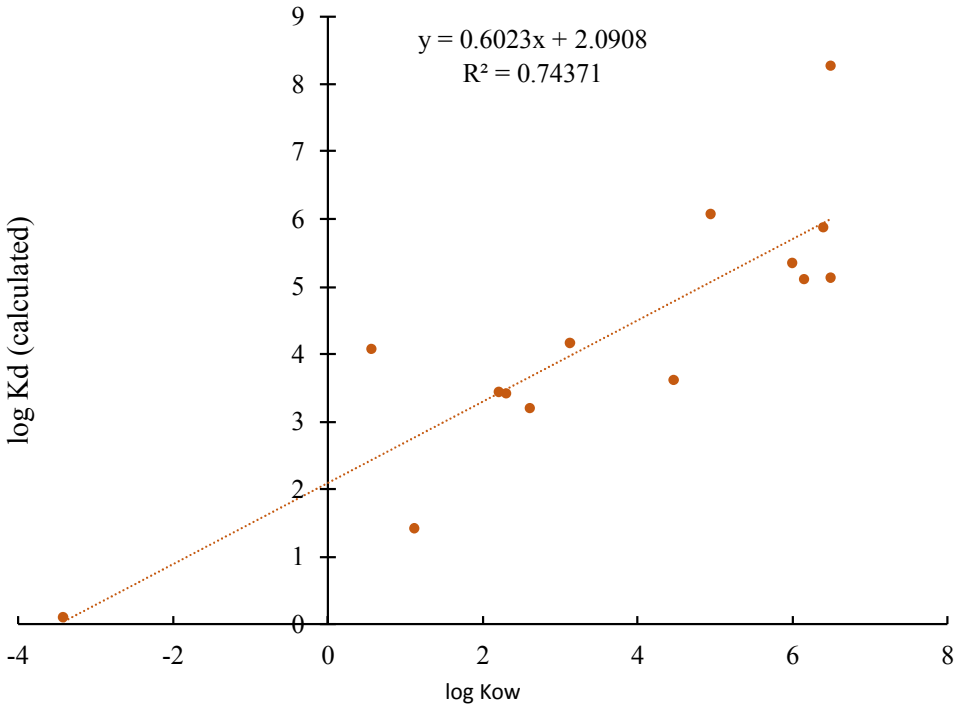

Figure S7. Correlation between K_{ow} and DMD simulated K_d values for Ceria nanoparticles