

Supplementary Information

Can COFs Replace MOFs in Flue Gas Separation? High-Throughput Computational Screening of COFs for CO₂/N₂ Separations

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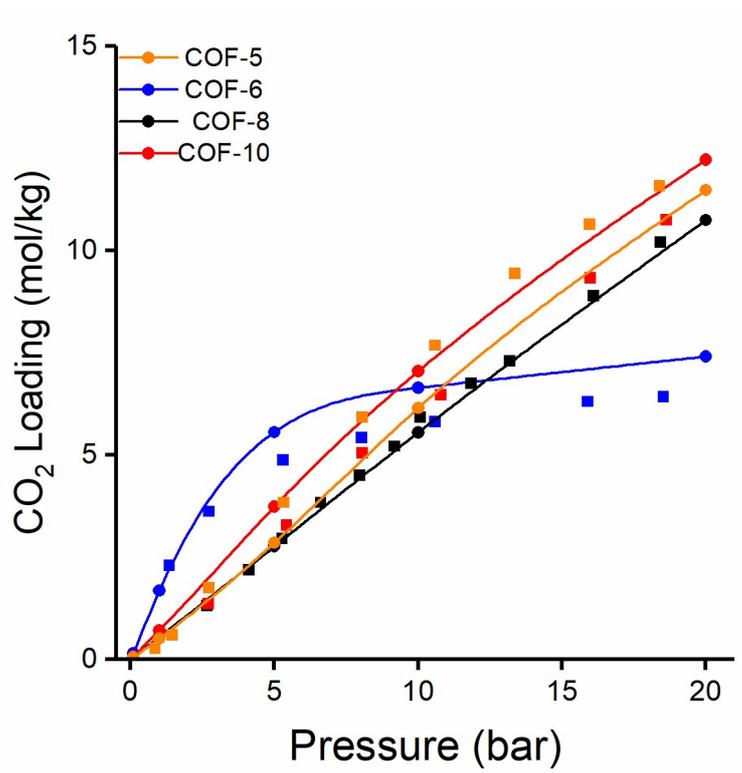


Figure S1. Comparison of experimental (squares) and simulated (lines) CO₂ adsorption isotherms of COFs at 298 K.

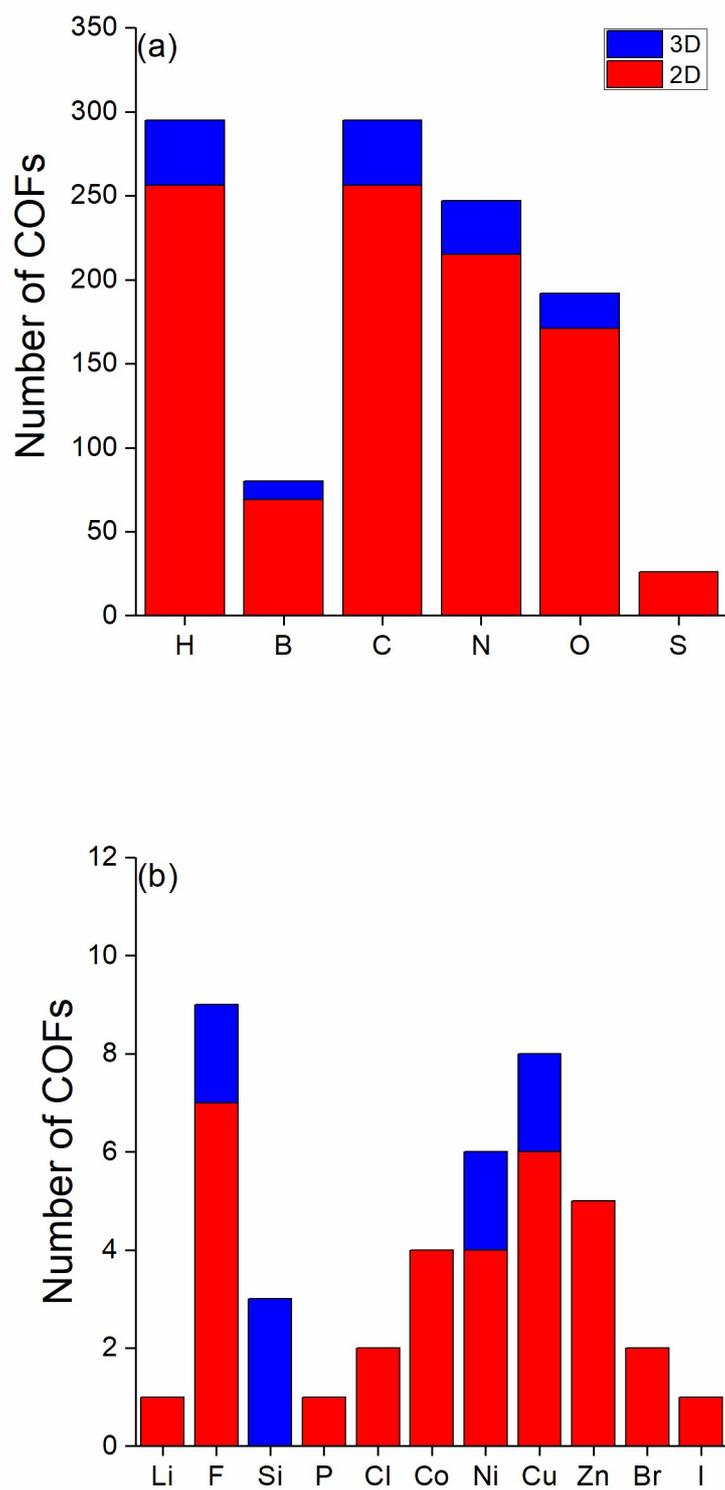


Figure S2. Distribution of (a) common atoms and (b) other atoms for the 295 COFs in CoRE COF database that we used.

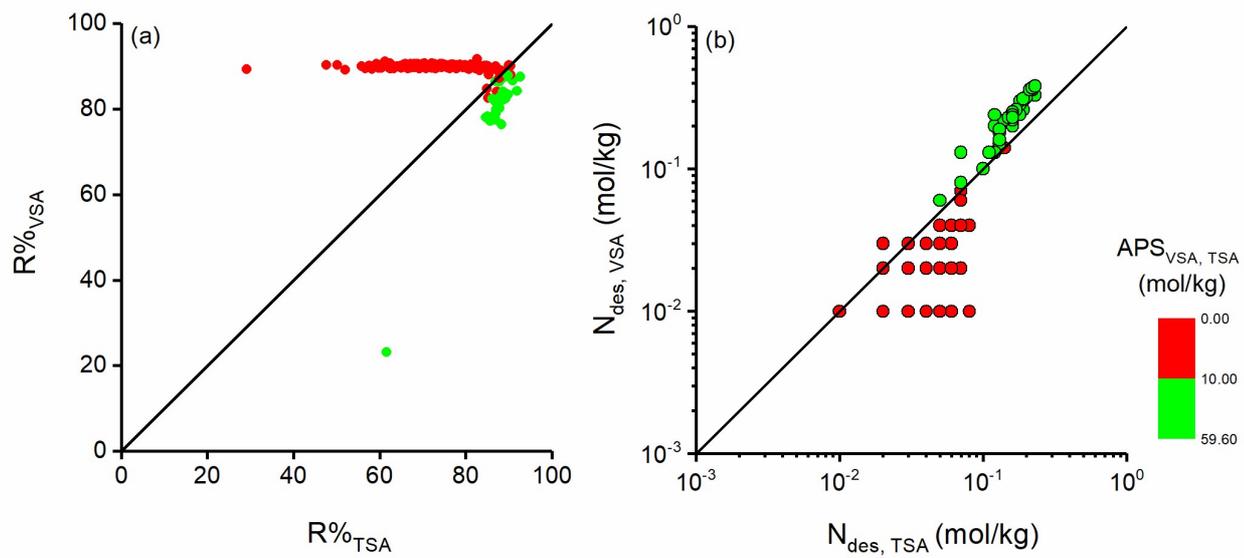


Figure S3. Comparisons of (a) R% (b) gas loadings at the desorption conditions of VSA and TSA processes.

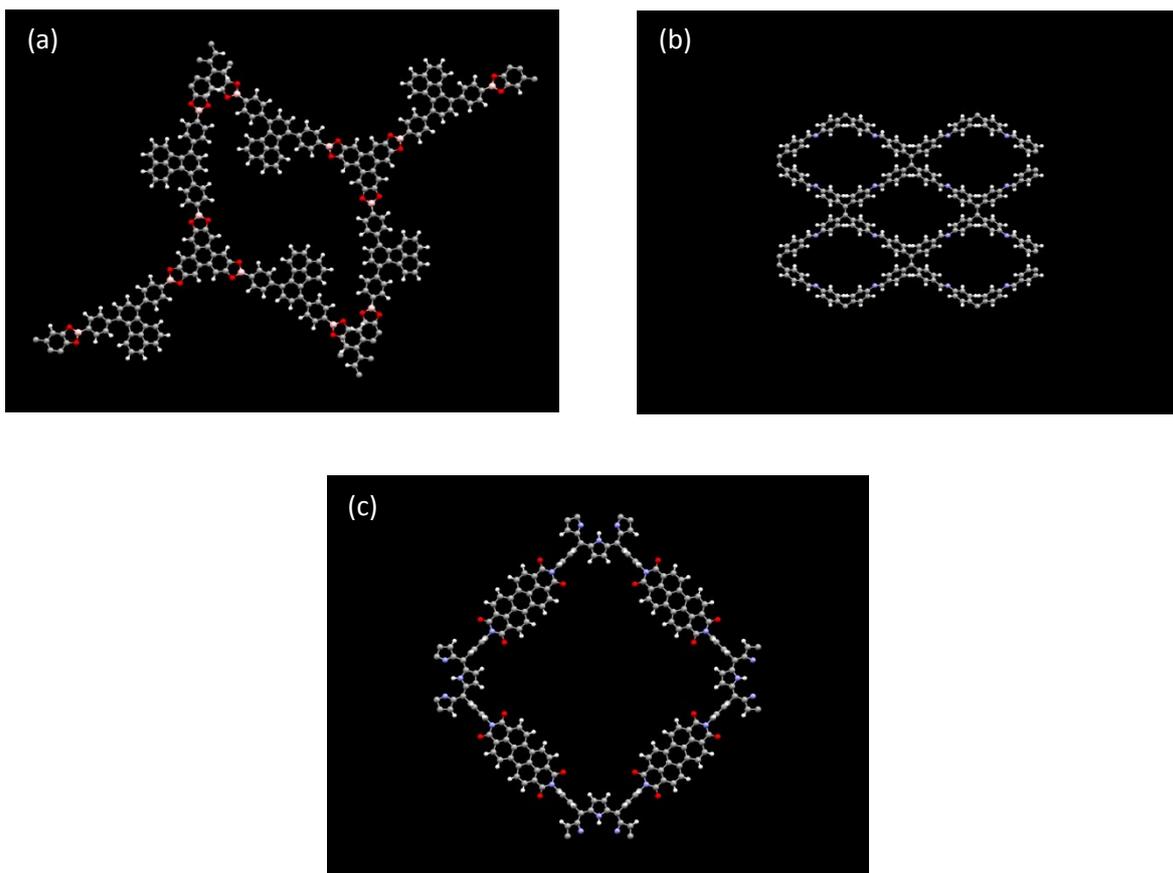


Figure S4. Unit cell representation of the most promising COFs in c direction: (a) FLT-COF-1 Staggered for VSA condition, (b) TPE-COF-1 for PSA condition and (c) PI-COF for TSA condition. Carbon: gray, oxygen: red, nitrogen: blue, hydrogen: white, boron: pink.

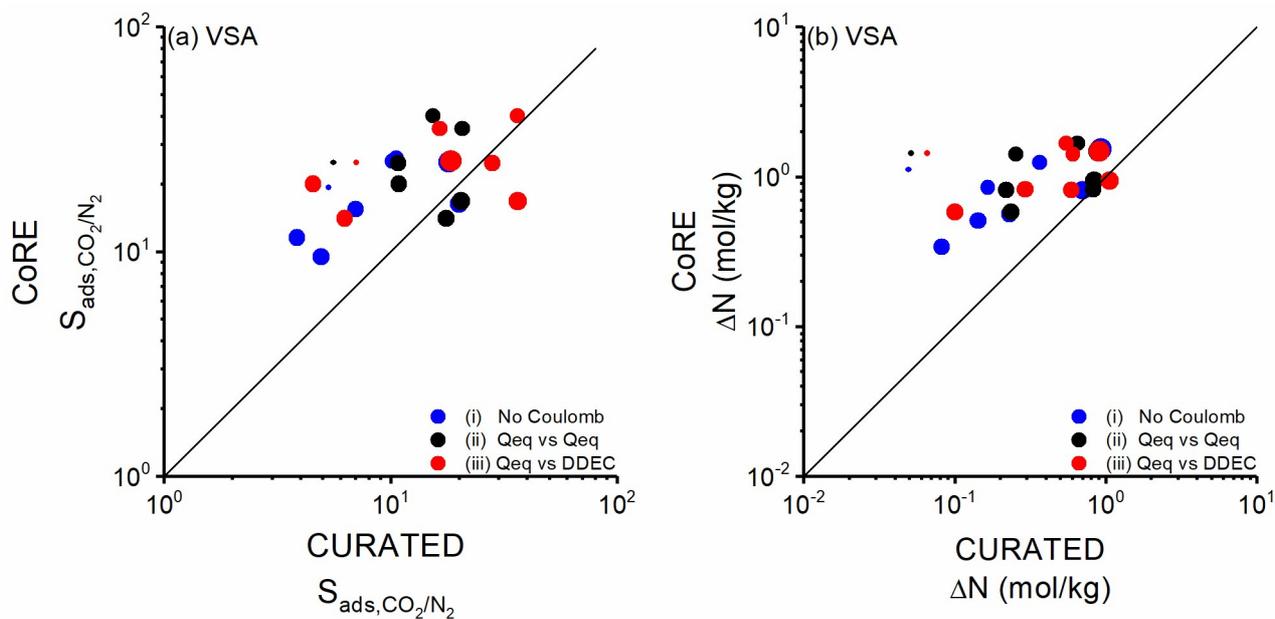


Figure S5. Comparisons of (a) S_{ads} (b) ΔN values of CURATED and CoRE COFs at VSA condition are shown. Symbols are sized based on $\frac{ASA_{\text{CURATED}}}{ASA_{\text{CoRE}}}$ while the normal size of the symbols can be seen in the legend.

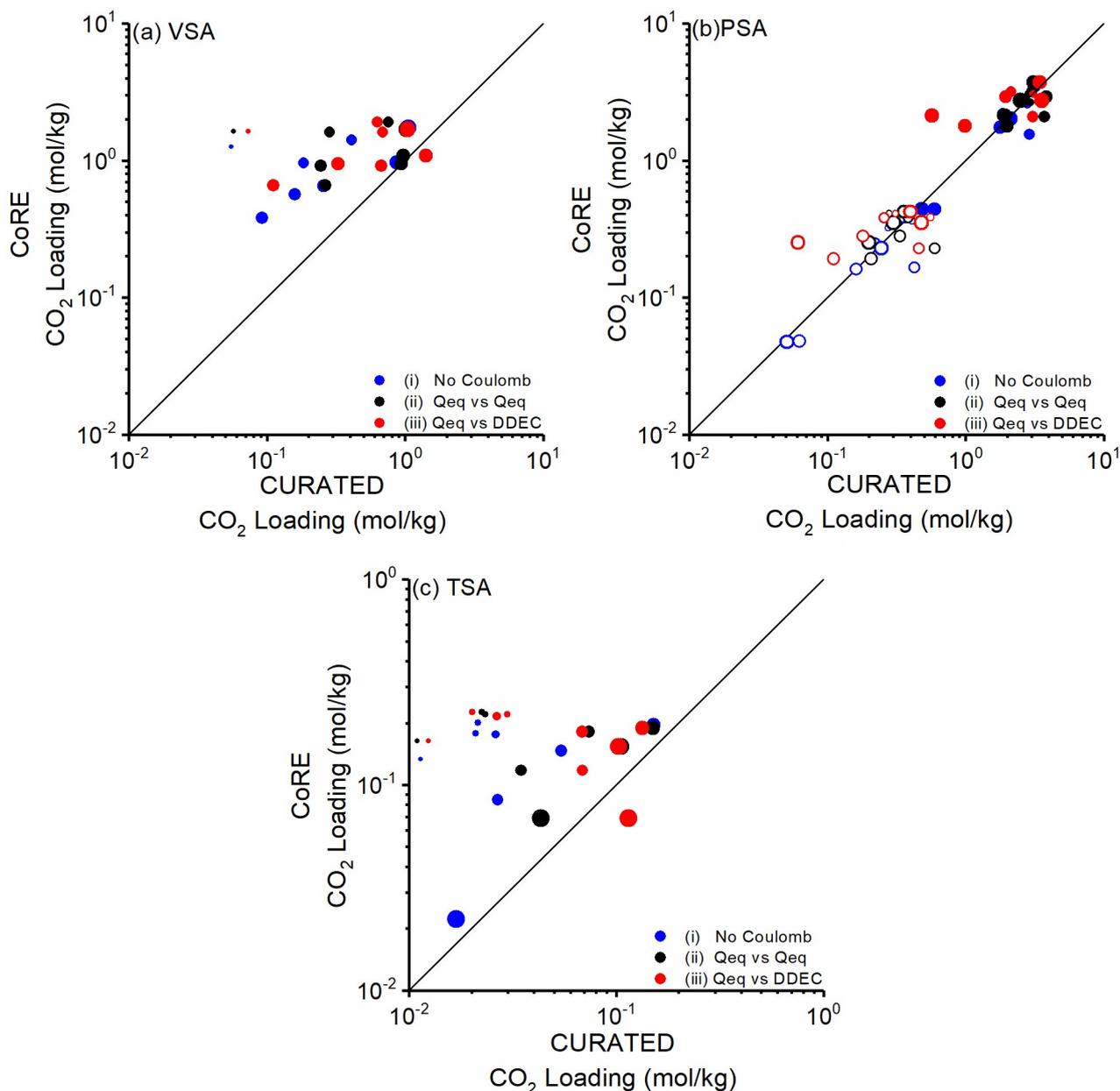


Figure S6. Comparisons of CO₂ loading values of CURATED and CoRE COFs at (a) VSA, (b) PSA, and (c) TSA condition are shown. Symbols are sized based on $\frac{ASA_{CURATED}}{ASA_{CoRE}}$ while the normal size of the symbols can be seen in the legend. Hollow symbols in (b) represent the performances of top COFs identified for PSA process at VSA conditions.

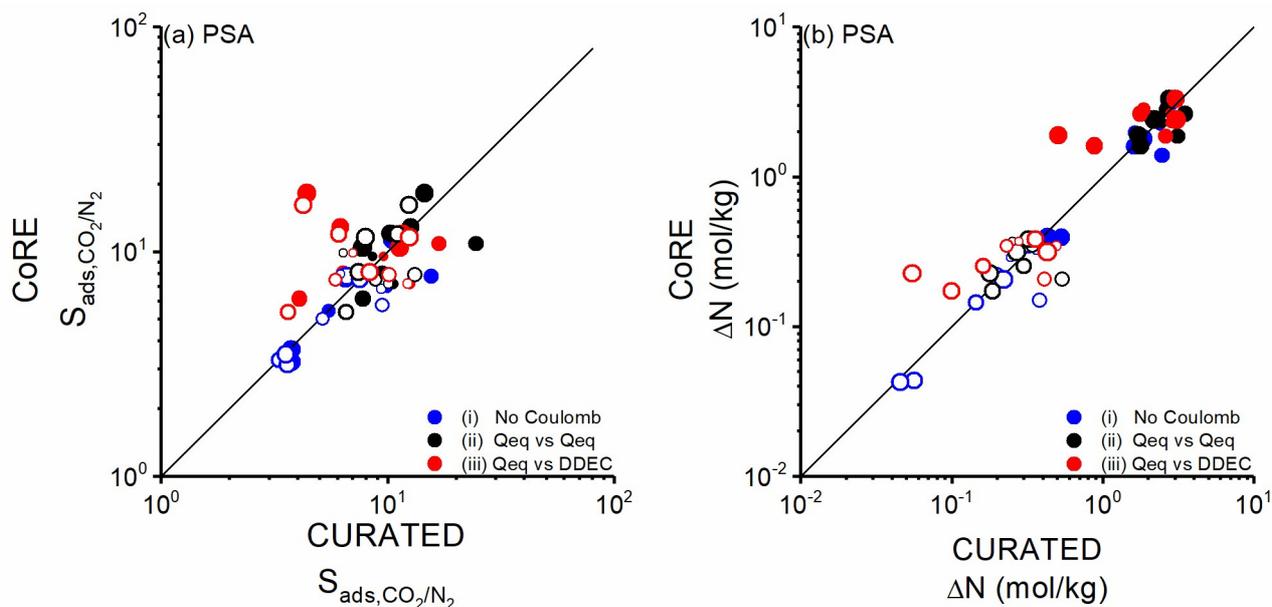


Figure S7. Comparisons of (a) S_{ads} (b) ΔN values of CURATED and CoRE COFs at PSA condition are shown. Symbols are sized based on $ASA_{\text{CURATED}}/ASA_{\text{CoRE}}$ while the normal size of the symbols can be seen in the legend. Hollow symbols represent the performances of top COFs identified for PSA process at VSA conditions.

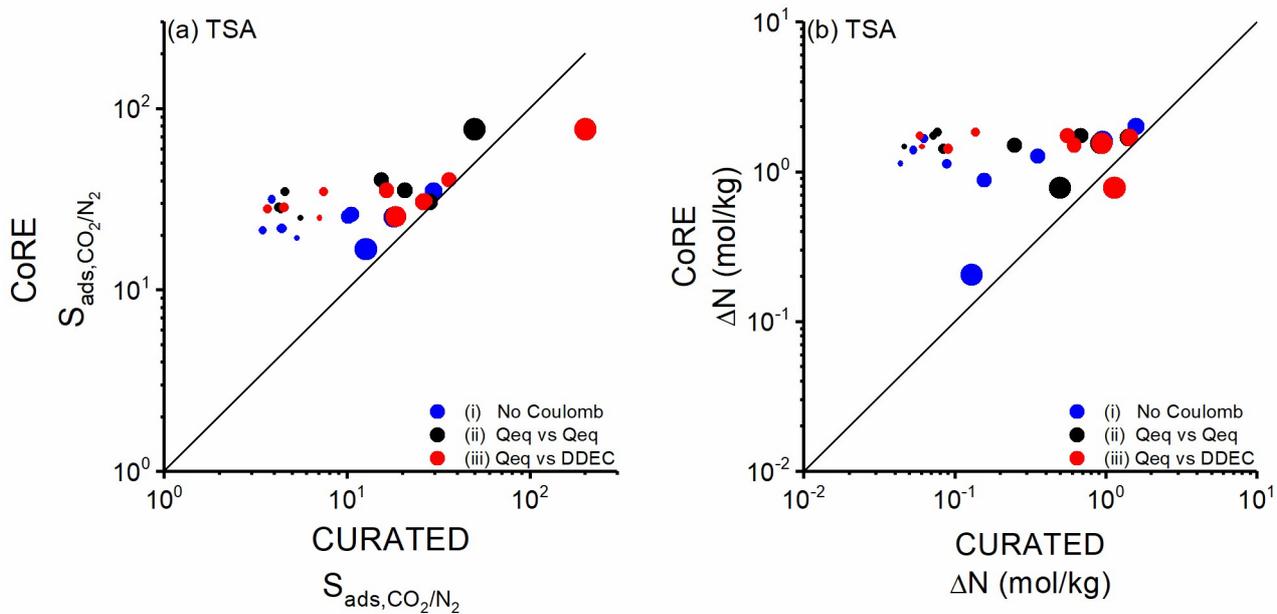


Figure S8. Comparisons of (a) S_{ads} (b) ΔN values of CURATED and CoRE COFs at TSA condition are shown. Symbols are sized based on $ASA_{\text{CURATED}}/ASA_{\text{CoRE}}$ while the normal size of the symbols can be seen in the legend.

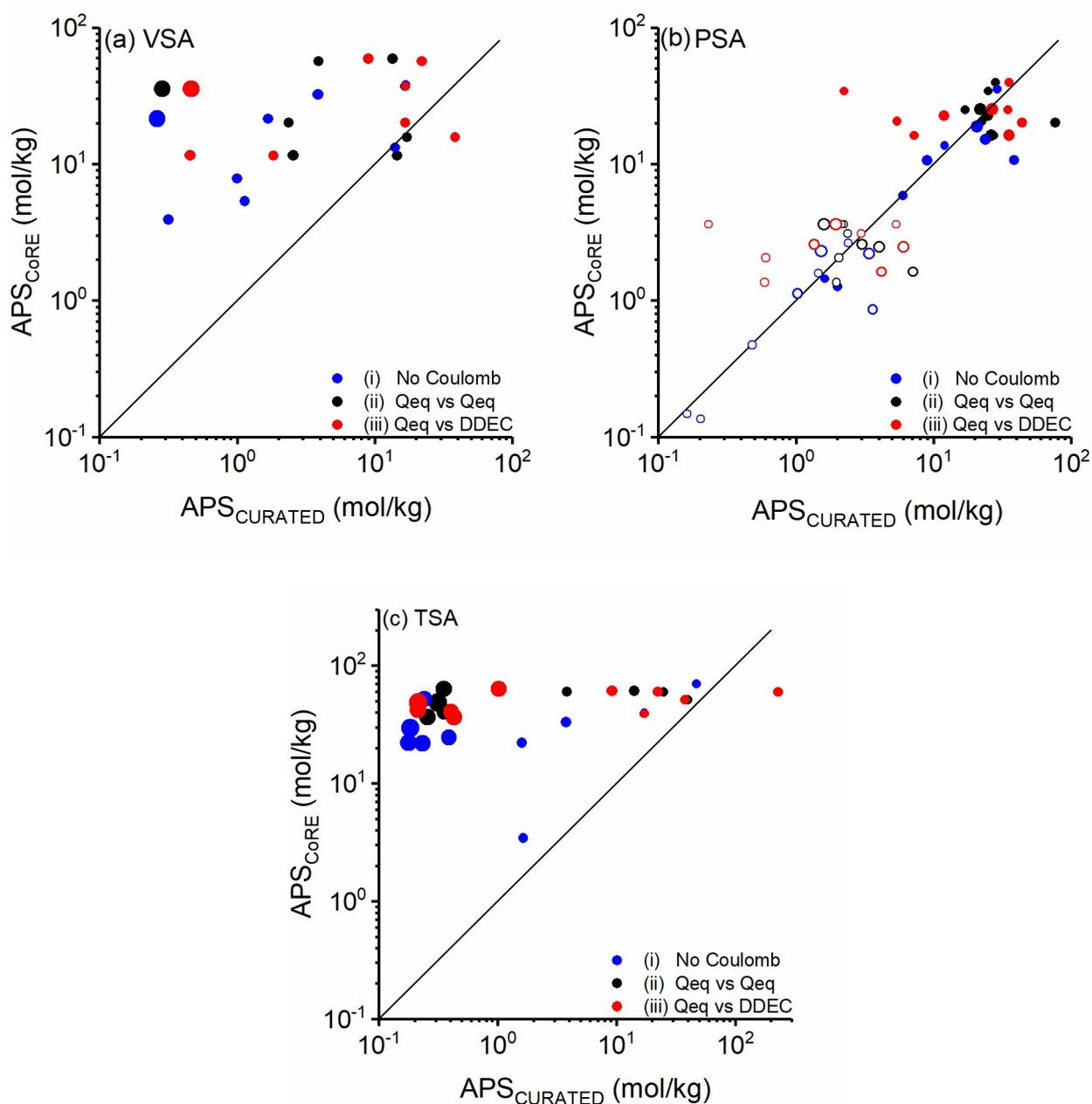


Figure S9. Comparisons of APSs of CURATED and CoRE COFs at (a) VSA, (b) PSA, and (c) TSA conditions. Symbols are sized based on $\rho_{CURATED}/\rho_{CoRE}$ while the normal size of the symbols can be seen in the legend. Hollow symbols in (b) represent the performances of top COFs identified for PSA process at VSA conditions.

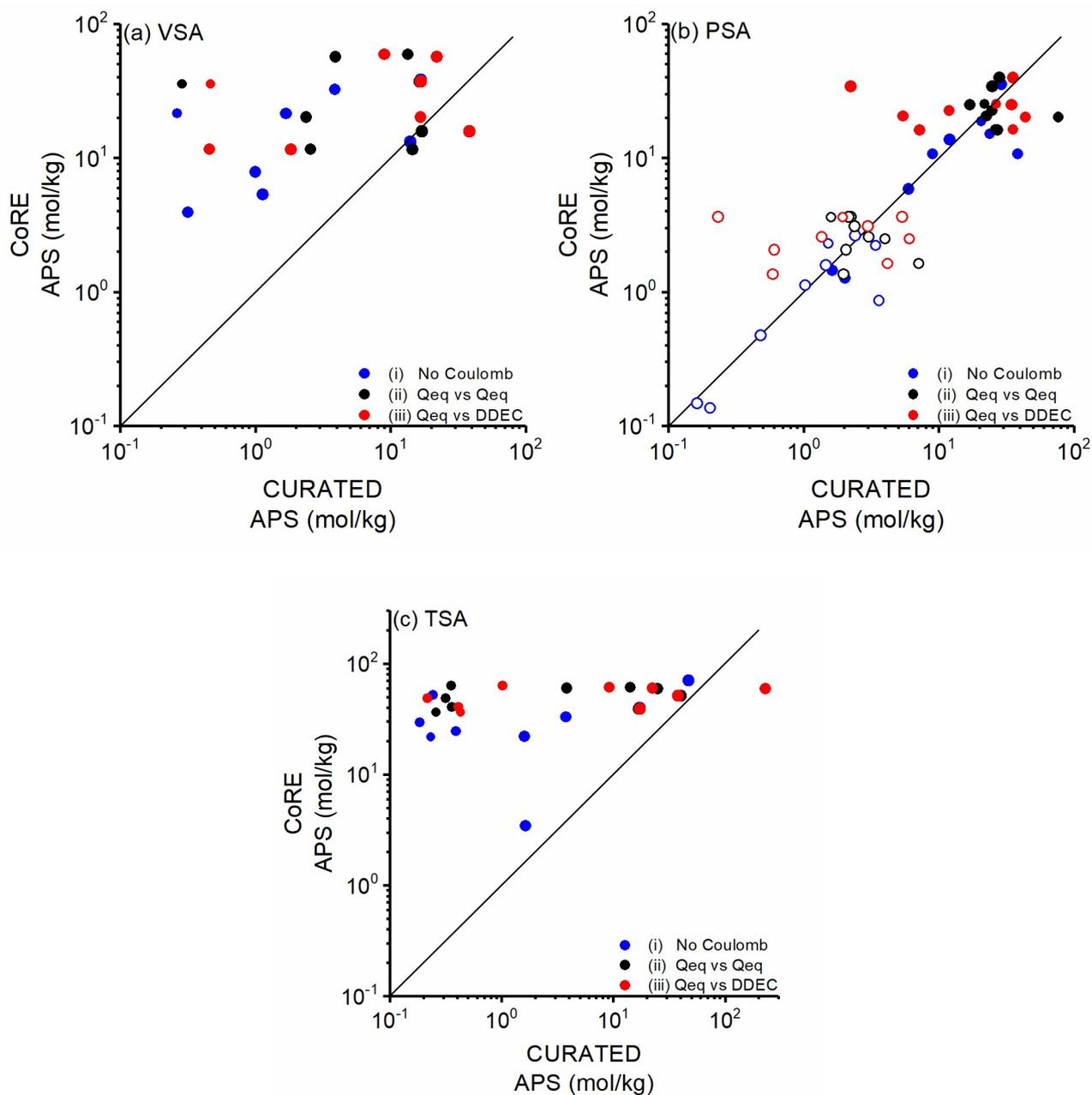


Figure S10. Comparisons of APSs of CURATED and CoRE COFs at (a) VSA, (b) PSA, and (c) TSA conditions. Symbols are sized based on $\phi_{\text{CURATED}}/\phi_{\text{CoRE}}$ while the normal size of the symbols can be seen in the legend. Hollow symbols in (b) represent the performances of top COFs identified for PSA process at VSA conditions.