



Figure SM3. Scatter plots of $\delta g^{inter/intra}$ (a.u.) versus $Sign(\lambda_2)\rho$ (a.u.) of some PDPA-water complexes, including PDPA-CH₃.H₂O, PDPA-Cl.H₂O, PDPA-F.H₂O, and PDPA-CN.H₂O. The corresponding RGD maps are superimposed at the top right of each panel. The red dots correspond to the intermolecular interactions, while the black dots correspond to the intramolecular interactions.