



Figure SM4. RDG maps (left) and Scatter plots of  $RDG (a.u.)$  versus  $Sign(\lambda_2)\rho (a.u.)$  of some PDPA-water complexes, including PDPA-H.H<sub>2</sub>O, PDPA-NH<sub>2</sub>.H<sub>2</sub>O, PDPA-CHO.H<sub>2</sub>O, and PDPA-NO<sub>2</sub>.H<sub>2</sub>O.