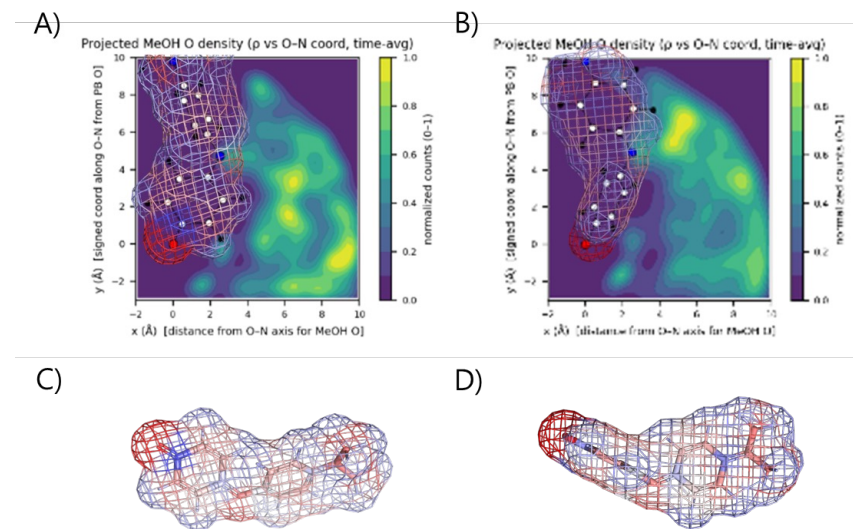


Simulation for excited structure of phenol blue (PB)

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- **Purpose:**
To determine the excited-state structure of PB through quantum chemical simulations
- **Approach:**
Comparison of time-resolved X-ray scattering data with theoretically calculated structures
- **Current Status:**
Multiple candidate structures have been identified; additional calculations are in progress to explore a broader structural landscape.

Computing system:	SQUID
hour	41599.79
job	1366.00



Figure, Solvent density and ESP of PB.

(a,b) Projected methanol oxygen density in the ground state (a) and u_3 (b).
(c,d) Corresponding ESP maps on the PB surface.