Title:	Design of Fluorescent and Robust Covalent Organic Framework Host Matrices for Illuminating Mechanistic Insight into Solvatochromic Decoding
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Abstract:	Two functional covalent organic frameworks (COFs), constructed from 3-connected triazine-based amine or hydrazine with linear dialdehyde, are decorated with molecular docking sites to showcase their solvatochromic decoding behavior toward volatile solvent molecules (VSMs). These luminescent and crystalline COFs, namely, COF-N and COF-NN, are characterized by numerous analytical techniques. After accommodation of different VSMs as guests, the inclusion compounds of COF-N and COF-NN display solvatochromism. More fascinatingly, the singlet energy, band gaps, and lifetime of these VSM-accommodated COF-N and COF-NN are linearly correlated with the properties of VSMs. Density functional theory (DFT) and Monte Carlo simulation studies further support the interaction of VSMs with COF-N and COF-NN. The presence of an extra amine functionality in COF-NN leads to the better interaction with VSMs and, therefore, results in different modes of interaction and correlation. Considering their inestimable chemical diversity, this study introduces a new path for finely tuned solvatochromic properties by COFs.
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