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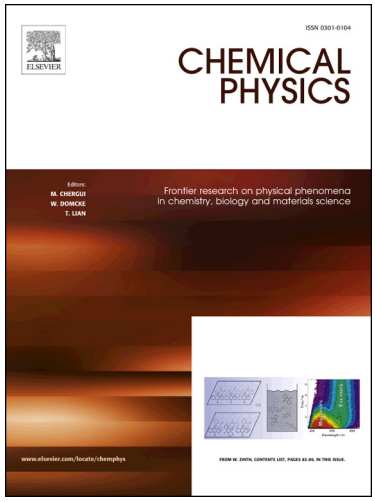

Specific solvent effect on the photophysical behavior of substituted chromones: A combined fluorescence, DFT and MD study

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Specific solvent effect on the photophysical behavior of substituted chromones: A combined fluorescence, DFT and MD study

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Abstract

Solvent dependent photophysical properties of two chromone derivatives, namely 7-amino-2-methyl chromone (AMC) and 3-cyano chromone (CyC), were studied by time-resolved fluorescence spectroscopy, density functional theory (DFT) calculation and molecular dynamics (MD) simulation. Contributions from different solvatochromic parameters were quantitatively estimated using Lippert-Mataga relation, uni-parametric $E_T(30)$ and multi-parametric Kamlet–Taft and/or Catalán relations. Notable solvatochromic shift in emission peak was estimated for CyC ($\Delta\lambda$ = 130 nm) in comparison with AMC ($\Delta\lambda$ = 53 nm). While both solvent hydrogen bond donation acidity and acceptance basicity is important in AMC photophysics, the latter is insignificant for CyC. Estimation of hydrogen bonding pattern in hydrated structures of AMC and CyC derived from MD simulation reveals that specific hydrogen bond donation of the solvent to carbonyl oxygen of the chromones is the most important microstructure modulating