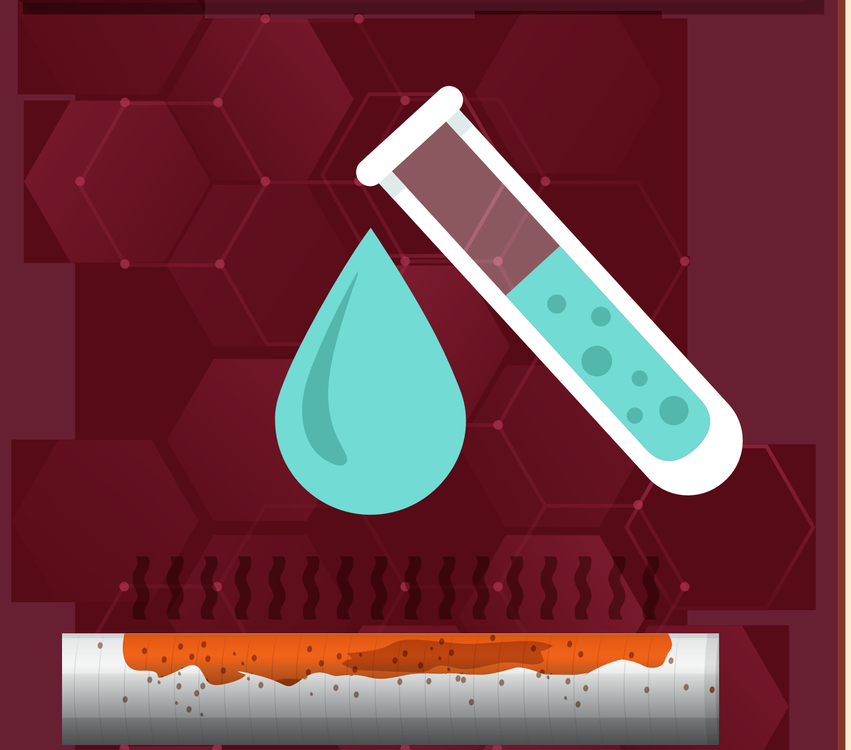
Molecular Simulations Reveal Strong Interactions Between Thiophene and Ionic Liquid Anions

RSC Advances

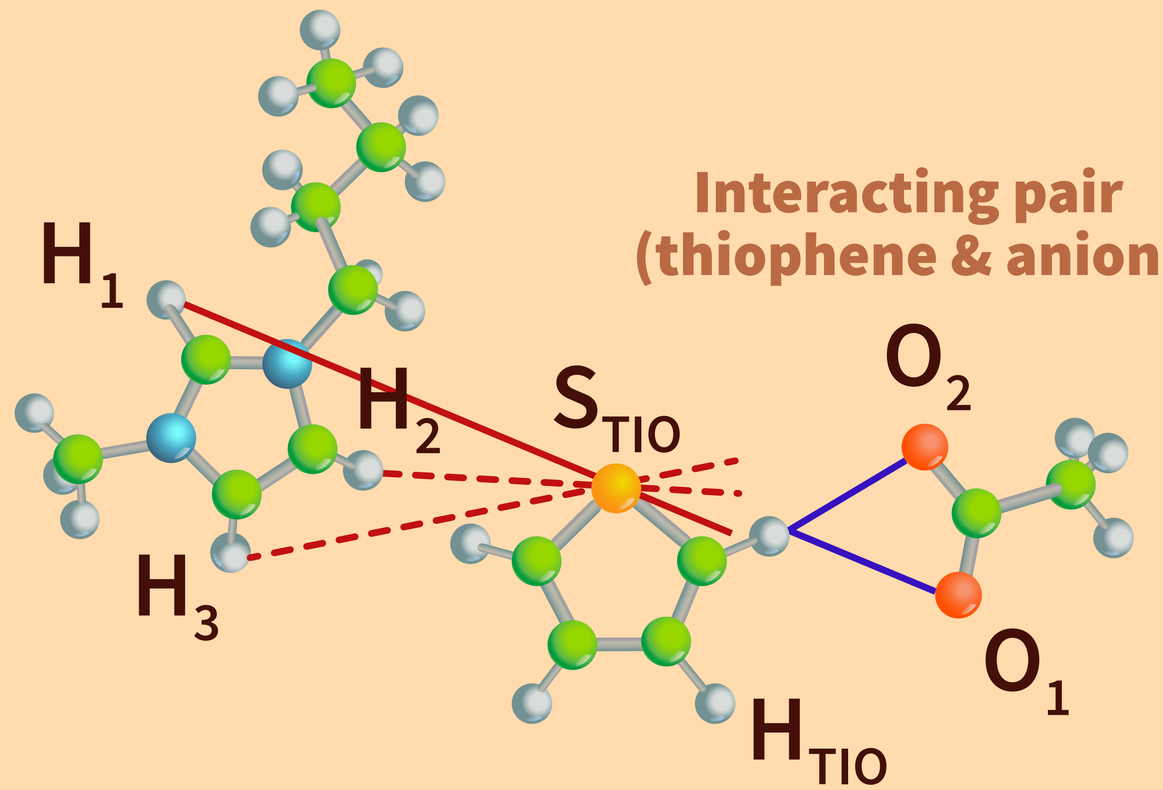
Sulphur compounds such as thiophenes trigger corrosion



Although green solvents such as ionic liquids (ILs) are used for thiophene extraction, the precise nature of interactions remains elusive

Can molecular simulations reveal the nature of interactions between thiophene and ILs?

- Excess chemical potentials ($\mu i^{E,\infty}$) at 300 and 343.15 K: $[C_4mim][CH_3COO] > [C_4mim][BF_4] > [C_4mim][Br] > [C_4mim][Cl]$



- Thiophene interacts with the IL anions (via H-bonding) at smaller distances in comparison with the IL cation
- Thiophene exhibits the strongest interactions with the anions and weakest with the cations of ILs

The favourable interactions between thiophene and IL anions hold promise for efficient and environment friendly desulphurisation

Excess chemical potential of thiophene in [C4MIM] [BF4, Cl, Br, CH3COO] ionic liquids, determined by molecular simulations
Gallo et al. (2021) | RSC Advances | DOI: 10.1039/d1ra04615b

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