Supplementary Information

Hierarchical study of mono- and multicharged imidazolium encapsulation in $p$-sulfonatocalix[4]arene molecular capsule

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Scheme 1. Synthesis of inclusion complexes 1 to 4.
Figure S1. (a-d) Fingerprint plots generated from the Hirshfeld surfaces mapped on 1-butylimidazolium (G1), 3,3’-(1,4-phenylenebis(methylene))bis(1-methylimidazolium) (G2), 3,3’,3”-(benzene-1,3,5-triytris(methylene))tris(1-methylimidazolium) (G3), and 3,3’,3”,3’’-(benzene-1,2,4,5-tetrayltetras(methylene))tetras(1-methylimidazolium) (G4) for complexes 1 to 4. (e) Relative percentage contributions of different interactions (C–H···H–C, C–H···O, C–H···C, C···C, C···O and other minor contacts) to the overall cations’ Hirshfeld surface.
Figure S2. (a-d) Fingerprint plots generated from the Hirshfeld surfaces mapped on \( p \)-sulfonatocalix[4]arene (SC4) for complexes 1 to 4. (e) Relative percentage contributions of different interactions (C–H···H–C, C–H···O, C–H···C, C···C, C···O, O···O and other minor contacts) to the overall SC4 Hirshfeld surface.