Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Electronic Supplementary Information: Phase and interface determination in computer simulations of liquid mixtures with high partial miscibility†

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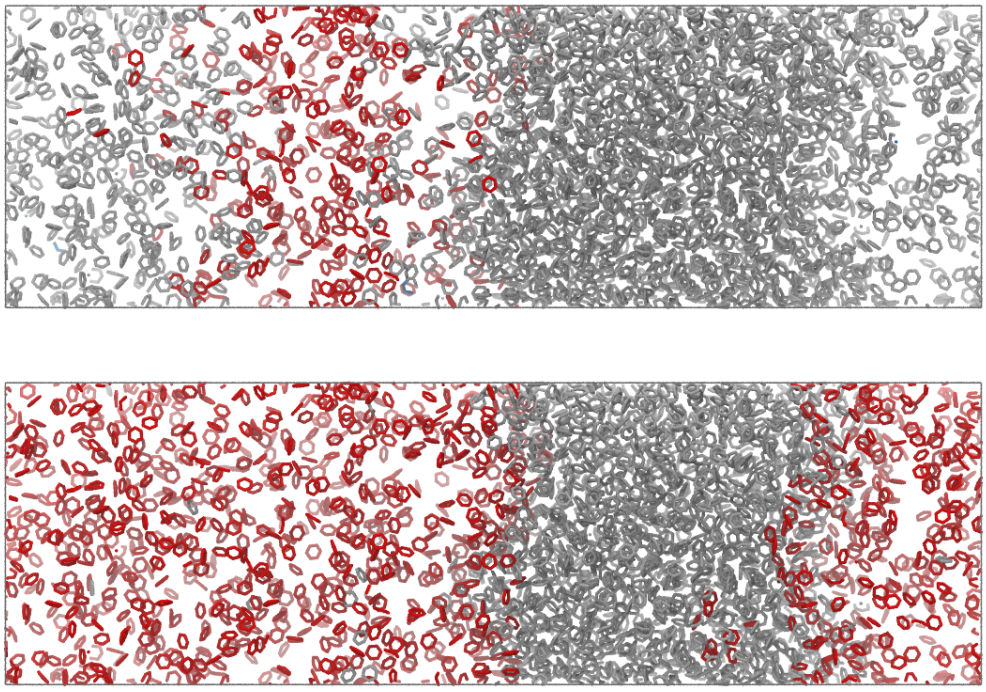

Fig. 1 Benzene molecules in one simulation snapshot of the BMIM NTf_2/benzene mixture, assigned to different phases using the simple clustering scheme and the ITIM algorithm (top) and the GITIM algorithm without any filtering (bottom). Gray: benzene-rich phase ; red: interfacial molecules of the benzene- rich phase.

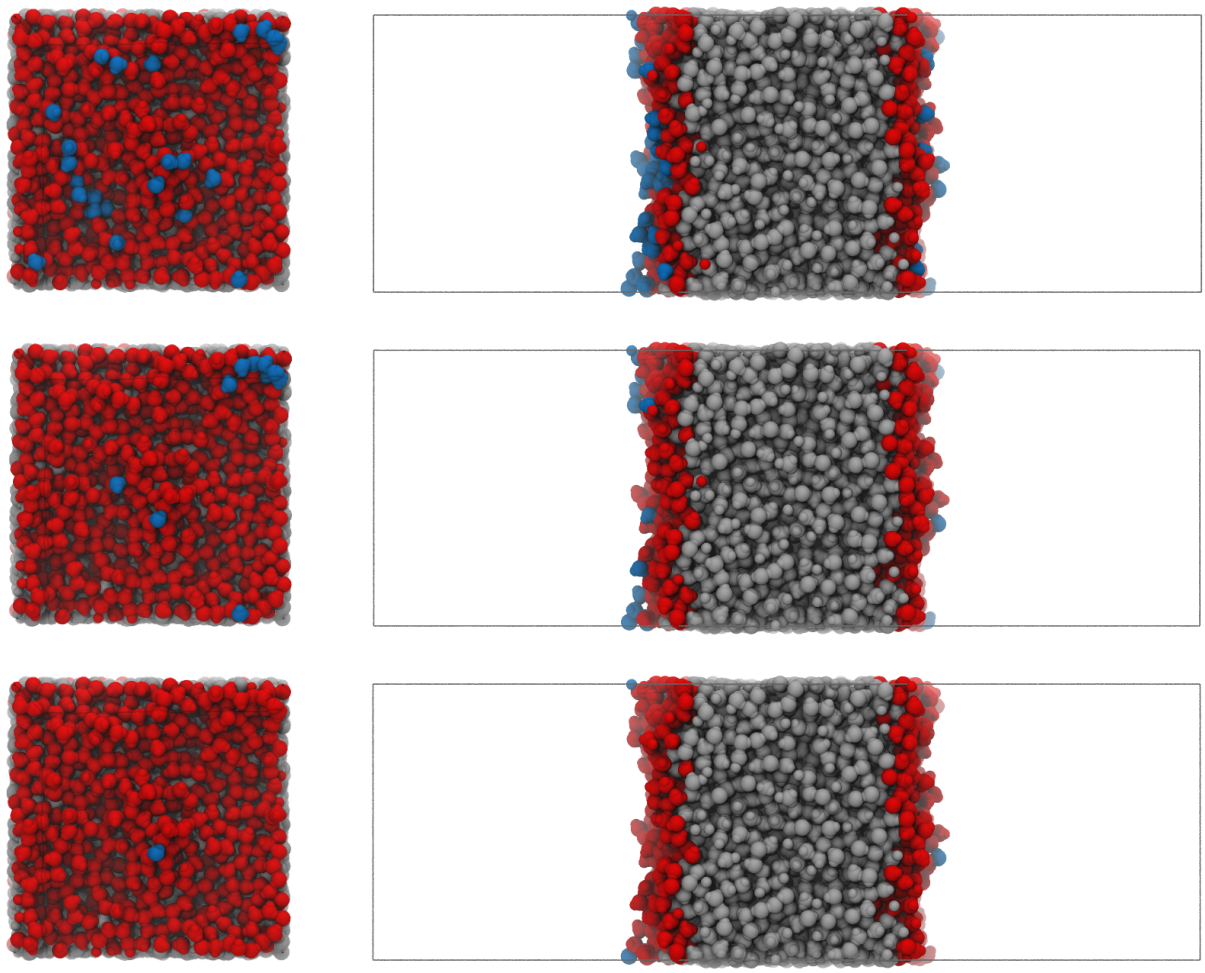

Fig. 2 Phase assignement using the automatic threshold determination in the limiting case of vanishing vapour pressure (SPC/E water/vapour interface at 300K) Gray: molecules assigned to the liquid phase ; red: interfacial molecules of the liquid phase; blue: molecules assigned to the vapour phase.From top to bottom: cutoff radius $r_c = 0.8$, 1.0 and 1.5 nm.