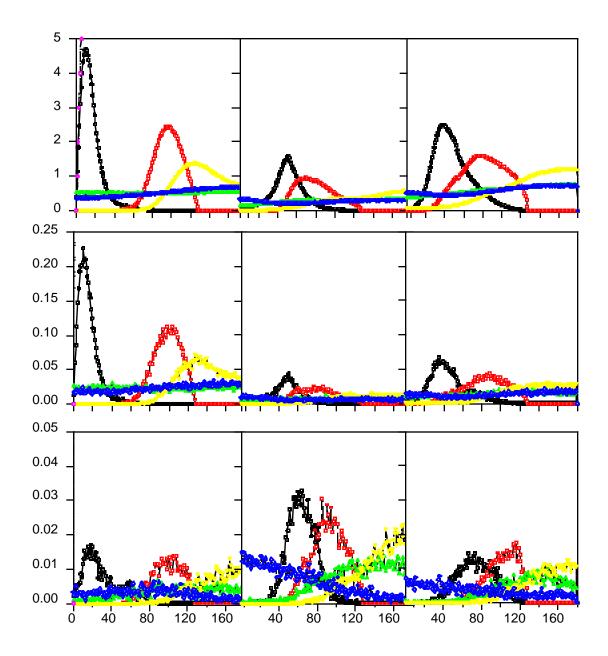
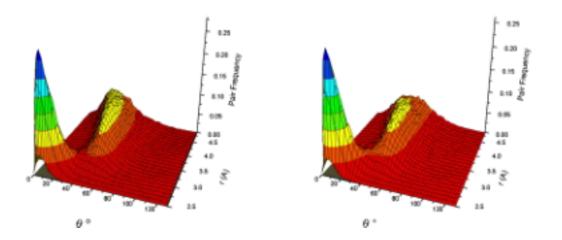
## A new angle on heat capacity changes in hydrophobic solvation (Supporting Information)

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Plots of  $\theta$  ( $\bullet$ ) and the secondary water-water orientation angles  $\psi$  ( $\blacksquare$ ),  $\varphi$  ( $\blacktriangle$ ),  $\chi$  ( $\checkmark$ ), and  $\omega$  ( $\diamond$ ) at r=2.8Å (Left), 3.5Å (Center) and 4.4Å (Right) for pure water (Upper), 1<sup>st</sup>-1<sup>st</sup> shell of argon (Middle) and 1<sup>st</sup>-1<sup>st</sup> shell of K<sup>+</sup> (Lower)



 $\rho(r,\theta)$  plots for 1<sup>st</sup>-2<sup>nd</sup> shell waters pairs around argon and K<sup>+</sup>.