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Diffusivity crossover and liquid-liquid transition in solutions of hard spheres in Jagla particles DARIO CORRADINI, Center for Polymer Studies and Department of Physics, Boston University, 590 Commonwealth Avenue, Boston, Massachusetts 02215, USA, PAOLA GALLO, Dipartimento di Fisica, Universita' Roma Tre, Via della Vasca Navale 84, I-00146 Roma, Italy, SERGEY V. BULDYREV, Department of Physics, Yeshiva University, 500 West 185th Street, New York, New York 10033, USA, H. EUGENE STANLEY, Center for Polymer Studies and Department of Physics, Boston University, 590 Commonwealth Avenue, Boston, Massachusetts 02215, USA — We study by discrete molecular dynamics simulations the relation between the thermodynamics and the diffusive behavior in solutions of hard spheres in Jagla particles, close to their liquid-liquid critical point. For comparison, we also show the same properties in the bulk Jagla particles system. The hard spheres and the Jagla model are used as spherically symmetric potentials for small hydrophobic solutes in water. We find that the fragile to strong dynamic transition observed when studying the diffusive behavior is always coupled to the low density to high density liquid transition. Above the liquid-liquid critical pressure the diffusivity crossover happens exactly at the Widom line of the systems, where the thermodynamic response functions show maxima. Below the liquid-liquid critical pressure, the diffusivity crossover corresponds to the crossing of the limit of mechanical stability lines and it shows hysteresis when going from high to low temperatures or vice versa. These findings prove that the strong connection between dynamics and thermodynamics found for bulk Jagla particles persists in hydrophobic solutions for concentrations from low to moderate.

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