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Role of Van der Waals interactions in determining the structure of liquid tellurides[1] MATTHIEU MICOULAUT, HUGO FLORES-RUIZ, Paris Sorbonne Universités, VANESSA COULET, Universités Aix-Marseille, ANDREA PIARRISTEGUY, Universit Montpellier II, MARK JOHNSON, GABRIEL CUELLO, Institut Laue Langevin, ANNIE PRADEL, Universit Montpellier II — The simulation of tellurides using standard density functional (DFT) theory based molecular dynamics usually leads to an overestimation of the bond distances and a noticeable mismatch between theory and experiments when e.g. structure functions are being directly compared. Here, the structural properties of several compositions of Ge-Te and Ge-Sb-Te liquids are studied from a combination of neutron diffraction and DFT-based molecular dynamics. Importantly, we find an excellent agreement in the reproduction of the structure in real and reciprocal spaces, resulting from the incorporation of dispersion forces in the simulation. We then investigate structural properties including structure factors, pair distribution functions, angular distributions, coordination numbers, neighbor distributions, and compare our results with experimental findings.

References:

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