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A refined description of solid, liquid, and supercooled silicon with the SCAN density functional

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Despite silicon being of great technological importance, an understanding of its behavior across the phase diagram is still lacking, especially near liquid-solid coexistence. The difficulty in describing silicon near coexistence from first principles lies in discriminating between the metallic and covalent bonds present in the material. Using a newly developed density functional that can describe a wide variety of bonds with quantitative accuracy, we report a thorough investigation of liquid silicon in the vicinity of liquid-solid coexistence using ab initio molecular dynamics simulations. We observe a structural transition in the supercooled regime that is rooted in a change in the electronic structure of the material. We predict this transition to occur at a much higher temperature than previous first principles predictions, in line with our predictions of a higher melting point than previously computed, which also agrees better with experiments. We also discuss implications of the observed change in interatomic interactions for empirical models of transitions between two distinct liquids.