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Origin of line tension for a Lennard-Jones nanodroplet JOOST H. WEIJS, Physics of Fluids, University of Twente, Enschede, ANTONIN MARC-HAND, Laboratoire de Physique et Mécanique des Milieux Hétérogènes, ES-PCI, Paris, JACCO H. SNOEIJER, Physics of Fluids, University of Twente, Enschede, BRUNO ANDREOTTI, Laboratoire de Physique et Mécanique des Milieux Hétérogènes, ESPCI, Paris, DETLEF LOHSE, Physics of Fluids, University of Twente, Enschede — The existence and origin of line tension has remained controversial in literature. To address this issue we compute the shape of nanodrops using molecular dynamics and compare them using density functional theory in the approximation of the sharp kink interface. We show that the deviation from Young's law is very small and would correspond to a typical line tension length scale (defined as line tension divided by surface tension) similar to the molecular size. It turns out that, for Lennard-Jones droplets, line tension is always negative and most pronounced at small contact angles. We propose an alternative interpretation based on the geometry of the interface at the molecular scale.

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