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Melting of Simple Solids and the Elementary Excitations of the Communal Entropy ANGELO BONGIORNO, School of Chemistry and Biochemistry, Georgia Institute of Technology — The melting phase transition of simple solids is addressed through the use of atomistic computer simulations. Three transition metals (Ni, Au, and Pt) and a semiconductor (Si) are considered in this study. Iso-enthalpic molecular dynamics simulations are used to compute caloric curves across the solid-to-liquid phase transition of a periodic crystalline system, to construct the free energy function of the solid and liquid phases, and thus to derive the thermodynamical limit of the melting point, latent heat and entropy of fusion of the material. The computational strategy used in this study yields accurate estimates of melting parameters, it consents to determine the superheating and supercooling temperature limits, and it gives access to the atomistic mechanisms mediating the melting process. In particular, it is found that the melting phase transition in simple solids is driven by exchange steps involving a few atoms and preserving the crystalline structure. These self-diffusion phenomena correspond to the elementary excitations of the communal entropy and, as their rate depends on the local material cohesivity, they mediate both the homogeneous and non-homogeneous melting process in simple solids.

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