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**Thermodynamics of type-I and type-II Si clathrates: a computer simulation study**[1] CAETANO MIRANDA, MIT, ALEX ANTONELLI, Universidade Estadual de Campinas — Few years ago a guest free type-II clathrate of silicon was obtained. This new form of elemental silicon is remarkably stable up to high temperatures. It is now clear that in order to devise new synthesis routes for these materials a better understanding of their thermodynamic properties is highly desirable. In this work, we present a computational study, employing the isobaric Monte Carlo method, of the thermodynamic properties at zero pressure of different phases of silicon, namely, both clathrate forms, $Si_{46}$ (type-I) and $Si_{34}$ (type-II), diamond crystalline silicon, liquid silicon, and amorphous silicon ($a$-Si). The Gibbs free energies, calculated by the reversible scaling method, allow us to determine the stable and metastable relations between these various phases. We have found the melting point of $Si_{46}$ and $Si_{34}$ clathrate structures to be at $1482 \pm 25$ K and $1522 \pm 25$ K, respectively. Our result for the melting point of $Si_{34}$ is in good agreement with the experimental value of 1473 K. The results also indicate that both clathrate forms are more stable than $a$-Si for any temperature up to their melting point. Based on our findings we discuss the feasibility of routes for the growth of these materials, such as solid-phase epitaxy and liquid-phase epitaxy.

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