PHYSIKALISCHES KOLLOQUIUM

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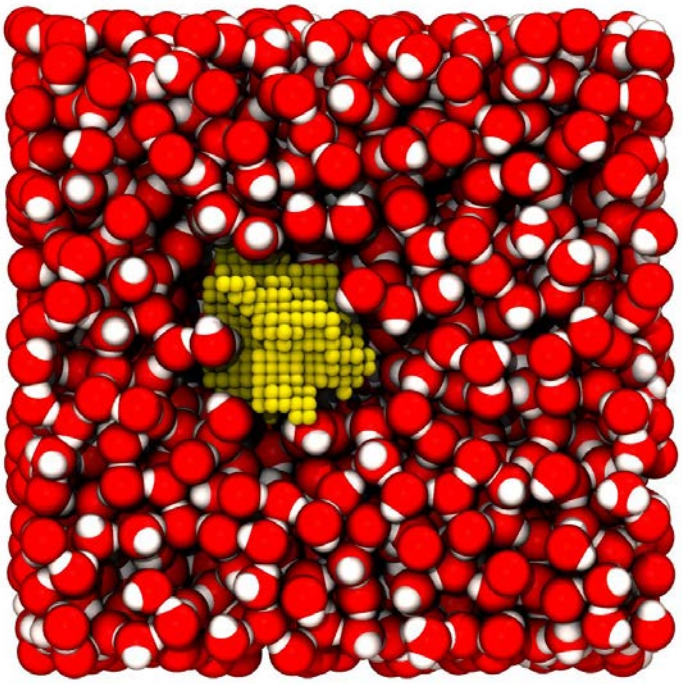
IM GROßEN HÖRSAAL



EXPLORING THE MECHANISM AND KINETCS OF NUCLEATION PROCESSES: FROM CRYSTALLIZATION TO CAVITATION

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Computer simulations of first order phase transitions occurring via nucleation and growth are demanding for several distinct but related reasons. Particularly close to coexistence, the free energy barrier separating the metastable from the stable phase can be high, leading to nucleation times that vastly exceed the time scales accessible to molecular dynamics simulations. Other difficulties arising in the simulation of nucleation processes consist in detecting local structures characteristic for the stable and metastable phases and in identifying the degrees of freedom that capture the essential physics of the transition mechanism. In this talk, I will discuss simulation approaches to address these problems, using the crystallization of supercooled liquids and cavitation of water under tension as illustrative examples.