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Ab Initio Calculations on Point Defect Thermodynamics in Nb_3Sn

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Point defects play a critical role in Nb_3Sn superconducting radio frequency (SRF) cavity physics. Using *ab initio* techniques, we can calculate key properties of defects including formation and interaction free energies, hopping barriers, and their effect on T_c. Here we will focus on the experimentally-relevant cases of antisite defects and oxygen and hydrogen interstitial impurities. Based on our results, we can better understand why defects may occur at high concentrations in the material as has been observed experimentally, and what the consequences of high defect concentrations might be for SRF performance. Furthermore, we consider how changes to the Nb_3Sn coating process could alter defect behavior in the growing layer, resulting in more homogeneous layers and better performance.

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