From models to mechanisms: defects and charge trapping in amorphous silicon nitride

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Stellingen
Behorende bij het proefschrift

From Models to Mechanisms:
Defects and Charge Trapping in Amorphous Silicon Nitride

i Crystalline proxies misrepresent amorphous silicon nitride because its behavior emerges from structural responses to charge injection or external defects as opposed to crystal-like point defects (Chapter 5-8).

ii Charge trapping is an intrinsic consequence of the density, network connectivity, and defect stability of amorphous silicon nitride. Thus, charge trapping is unavoidable (Chapter 5).

iii For structural models of amorphous materials, access to larger cells and longer trajectories outweighs the accuracy of first-principles methods (Chapter 3,4).

iv Statistical sampling is crucial for modeling disordered materials because rare local environments govern key properties (Chapter 3).

v Validation of amorphous models requires convergence across observables related to the question of research. Matching only a subset of observables inevitably produces systematic errors. (W. I. Choi *et al. Adv. Mater.* 2024, *36*, 2308054).

vi In materials design, disorder is a tunable variable rather than an imperfection. Thus, understanding inherent outliers is key for next-generation materials (Y. Liu *et al. Nat. Rev. Mater.* 2025, 228-241, 228-241).

vii Modeling without a mechanistic question produces numbers, not understanding. In computational chemistry, the 'why?' is more decisive than the 'how?' (A. Lambrecht *et al. Comput. Mater. Sci.* 2022, *211*, 111555).

viii In disordered materials, causal claims based on a small number of samples or global averages are meaningless (T. Nagahashi *et al. IEEE J. Electron Devices Soc.* 2025).

ix Doctoral curricula that prioritize specialization over breadth yield narrower researchers, thereby compromising their development towards well-rounded scholars.

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