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

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Stellingen
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*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.