

KEYNOTE PRESENTATION

Dr. Simon Elliott

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Dr Simon Elliott is a director at scientific software company Schrödinger. From 2001-2018 he led a research group at Tyndall National Institute, Ireland. Prior to that he studied chemistry in Trinity College Dublin and Karlsruhe Institute of Technology. He qualified as a Project Management Professional and is a Fellow of the Royal Society of Chemistry. He was co-chair of the 16th International Conference on Atomic Layer Deposition and chair of a 175-member COST network on the same topic.



"Concepts and Preconceptions - the Outlook for Simulations in ALD "

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Atomistic simulations in the field of atomic layer processing are introduced by looking at the key concepts - accuracy, speed, complexity, expertise, value - and our perceptions about them. We give recent examples of molecular and surface simulations that may challenge or reinforce those preconceptions.

The success of deposition and etch processes depends crucially on the properties of the precursor chemicals used, so that much innovation in this field centers around developing new precursors. The space of possible ligands is vast, much too large to be explored systematically in the lab. The area is therefore ripe for computational screening and design, as long as the relevant properties can be computed quickly and accurately. We discuss the quantifiable metrics for screening. For instance, a good precursor should show wide temperature windows for delivery and deposition, which can be related to reactivity and stability, which can in turn be computed to some extent at the molecular scale. We illustrate the points with a computational screening of zirconium precursors against thermal stability and nitride formation.

We also consider precursor volatility as a screening criterion and what makes it so difficult to simulate. Recent progress is reported in identifying its molecular basis and developing volatility models with machine learning, though many challenges remain. More generally, we discuss the emerging field of data science and potential benefits to the community if data can be better shared, curated and accessed.