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# Rebooting Materials Discovery and Design

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There are many challenges in atomic-scale materials modelling to quickening the pace and broadening the scope of impacts to real products in industrial research and development (R&D). These challenges require both the translators (or users) and developers of materials modelling software to rethink and "reboot" their approach with a renewed focus on ease-of-use and their experimental partners perspective to go beyond materials discovery to true materials design.

In industrial R&D translators need to reboot their knowledge base to include a deeper understanding of the day-to-day challenges of experimental partners and equipment. It is critical to anticipate the unexpected during formation, deposition, and bonding of materials to design simulation plans and methodologies to account for the inherent uncertainty in the manufacturing process. This perspective is especially important during the first engagement with small and large manufacturing companies exploring integrating materials models into their R&D flow. Through the translators' process of engaging with the experimentalist, they should provide an honest and thoughtful overview of both the power and limitations of the software. This ensures an effective collaboration and helps to improve the chances of success of the recommendations.

As an example, take the semiconductor industry's manufacture of integrated circuits (IC). In this industry "discovery" of a new material that meets a property target is only a small step in the design process. To introduce a new material into an IC manufacturing process it must survive physical interaction with 2 to 4 different processing techniques, bond across an interface with 1 to 4 materials, and function at varying thicknesses in different layers. This requires going beyond materials discovery to designing materials to survive a variety of topological, chemistry, thermal, and mechanical conditions. The translator must predict more than a single property, but property vectors that encompass as many potential complications as possible to maximize the chance of success. In practice this is often not computationally feasible with a one-step methodology and usually requires the translator's own engineering judgement and a funnel-type of methodology using varying levels of theory, tools, and material down-selection.

Materials modelling software developers also have a role to play in rebooting materials discovery and design. Look to the success and impacts of higher-level finite element tools in computational materials, circuit design, and CAD tools. Abaqus, AutoCAD, and Synopsys are successful at making broad impacts to industrial manufacturing and R&D. Their focus is on reliability of their software, providing a wide range of capabilities, and ease-of-use. They build tools and interfaces that automate much of the methodology and model setup decision-making process while ensuring a good standard of accuracy. A reboot of the software design and development process that incorporates this focus will serve materials modelling software developers well, while also enabling translators to increase the speed and scale of their impacts.