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New discovery tools for molecular materials design HEATHER KULIK, TERRY GANI, JON PAUL JANET, MIT — First-principles modeling has emerged as a critical component of materials screening and design, particularly for bulk systems with limited compositional degrees of freedom. However, strategies for molecular materials design have lagged behind the heterogeneous screening efforts, owing to the larger chemical space spanned by such molecular motifs. Aiming to overcome current limitations in molecular discovery, we present our recently introduced open-source molSimplify[1] toolkit. This software enables rapid, automated structure generation and discovery by building accurate geometries to enable high-throughput screening through a unique divide-and-conquer approach; it interfaces to multi-million-molecule databases to enable discovery; and we present recent strategies[2] adapted from the therapeutic drug design community to enable truly rational and iteratively-improved design strategies. Finally, we present our recent efforts on further acceleration of discovery both through high-throughput, high-quality guesses for transition states away from equilibrium and multi-resolution modeling using artificial neural networks with quantified uncertainty. [1]E. I. Ioannidis, T. Z. H. Gani, and H. J. Kulik "molSimplify: A toolkit for automating discovery in inorganic chemistry" *Journal of Computational Chemistry*, **37**, 2106-2117 (2016). [2]T. Z. H. Gani, E. I. Ioannidis, and H. J. Kulik "Computational Discovery of Hydrogen Bond Design Rules for Electrochemical Ion Separation" *Chemistry of Materials*, **28**, 6207-6218 (2016).

Heather Kulik
Massachusetts Inst of Tech-MIT

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