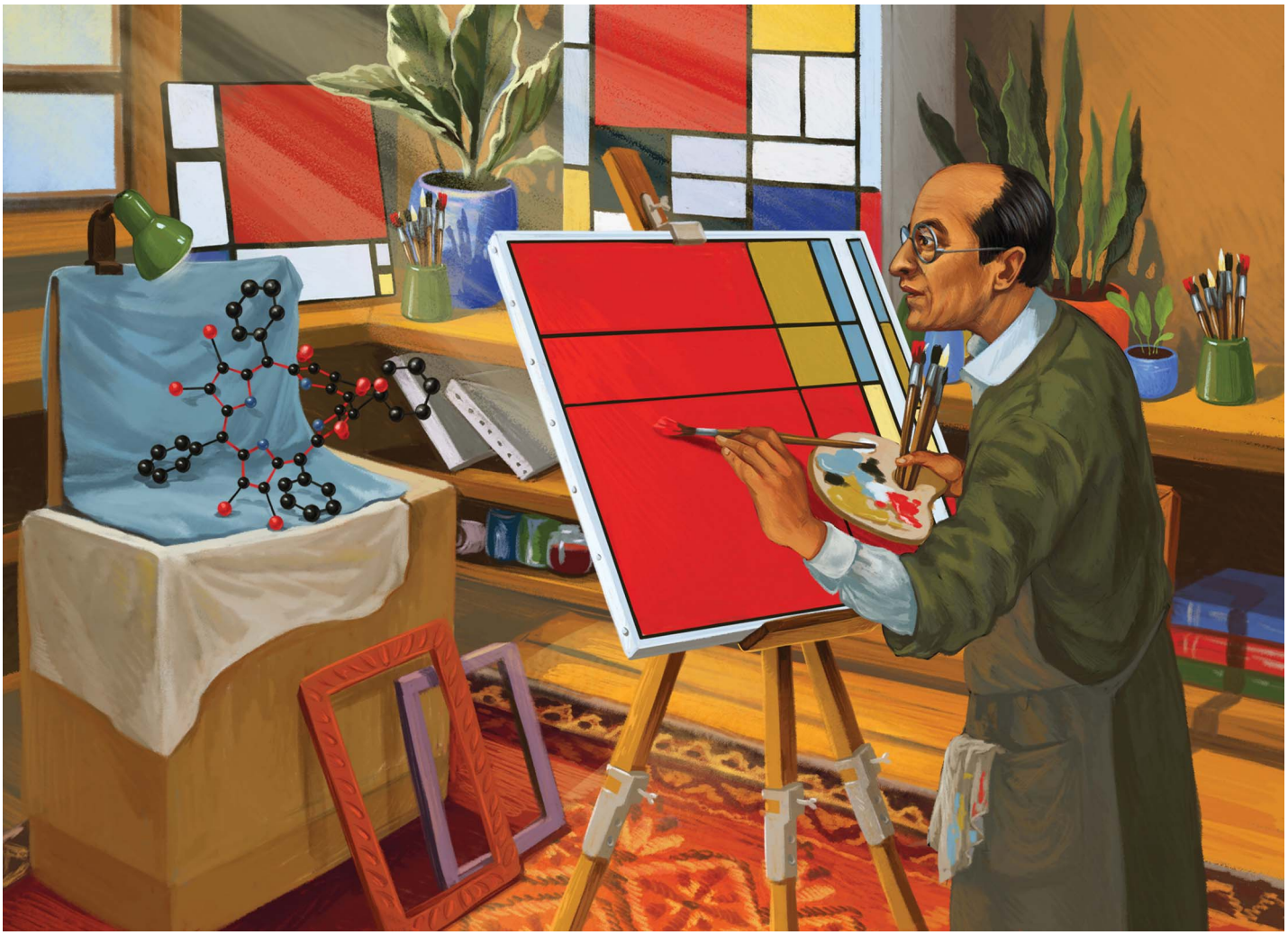

Showcasing research from Professor Senge's laboratory, School of Chemistry, Trinity College Dublin, Ireland and the Institute for Advanced Study, Technical University Munich, Germany.

Quantifying near-symmetric molecular distortion using symmetry-coordinate structural decomposition

SCSD is a new method and online toolset for analyzing crystal structures of molecules distorted from regular shape. Separating atom movements into symmetry modes, molecular conformation can be quantified and compared easily across databases, offering quantitative insight into the "molecular origami" approach to functional materials. Structural features can also be visualized by the program 'painting' the molecular conformations in the artistic De Stijl of Piet Mondrian.
Cover design by Ella Marushchenko.

As featured in:

See Christopher J. Kingsbury and Mathias O. Senge, *Chem. Sci.,* 2024, **15**, 13638.

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