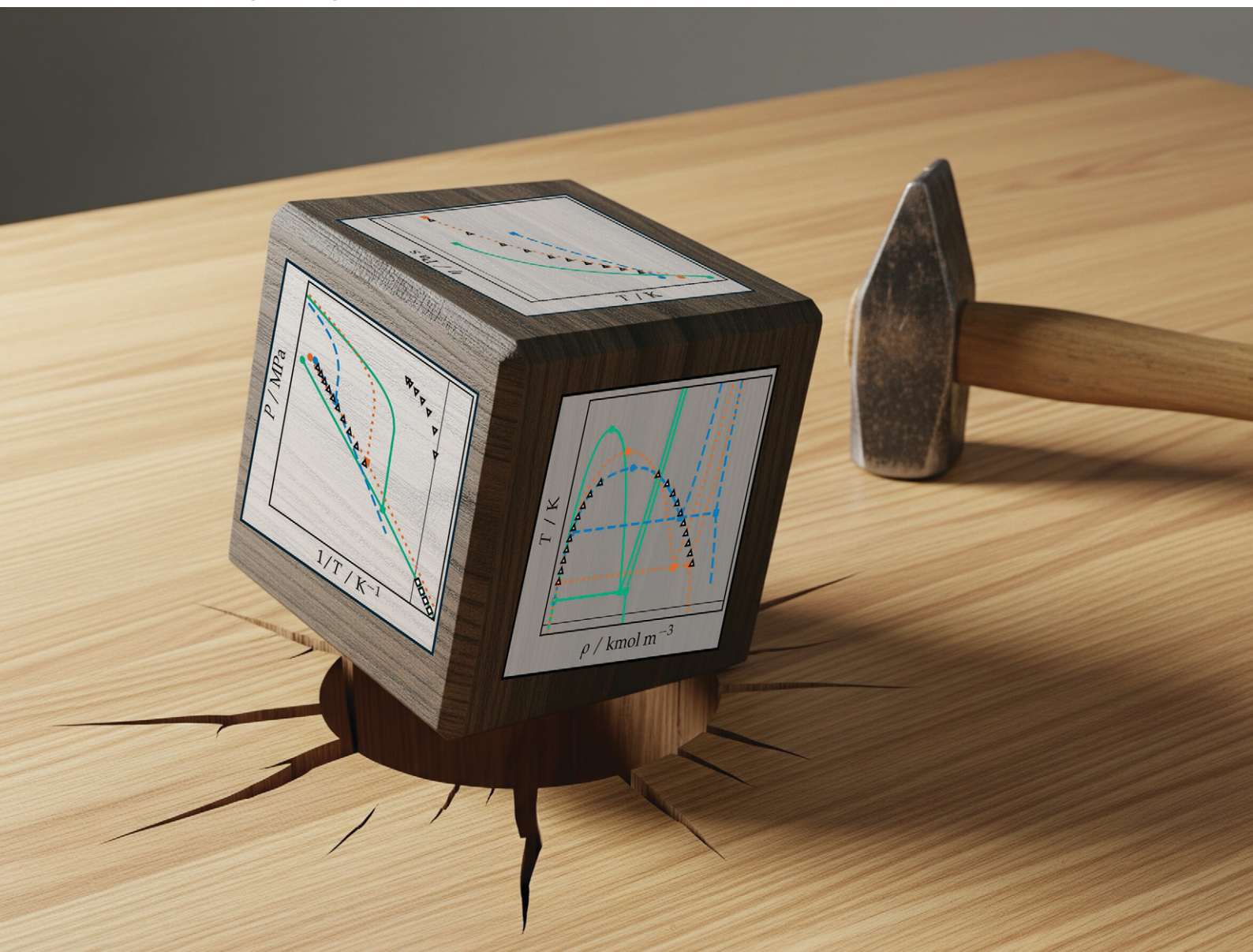


MSDE

Molecular Systems Design & Engineering

rsc.li/molecular-engineering



ISSN 2058-9689

PAPER

Gustavo Chaparro and Erich A. Müller
Fitting a square peg in a round hole: parameterisation of
quasi-spherical molecules employing the Mie potential