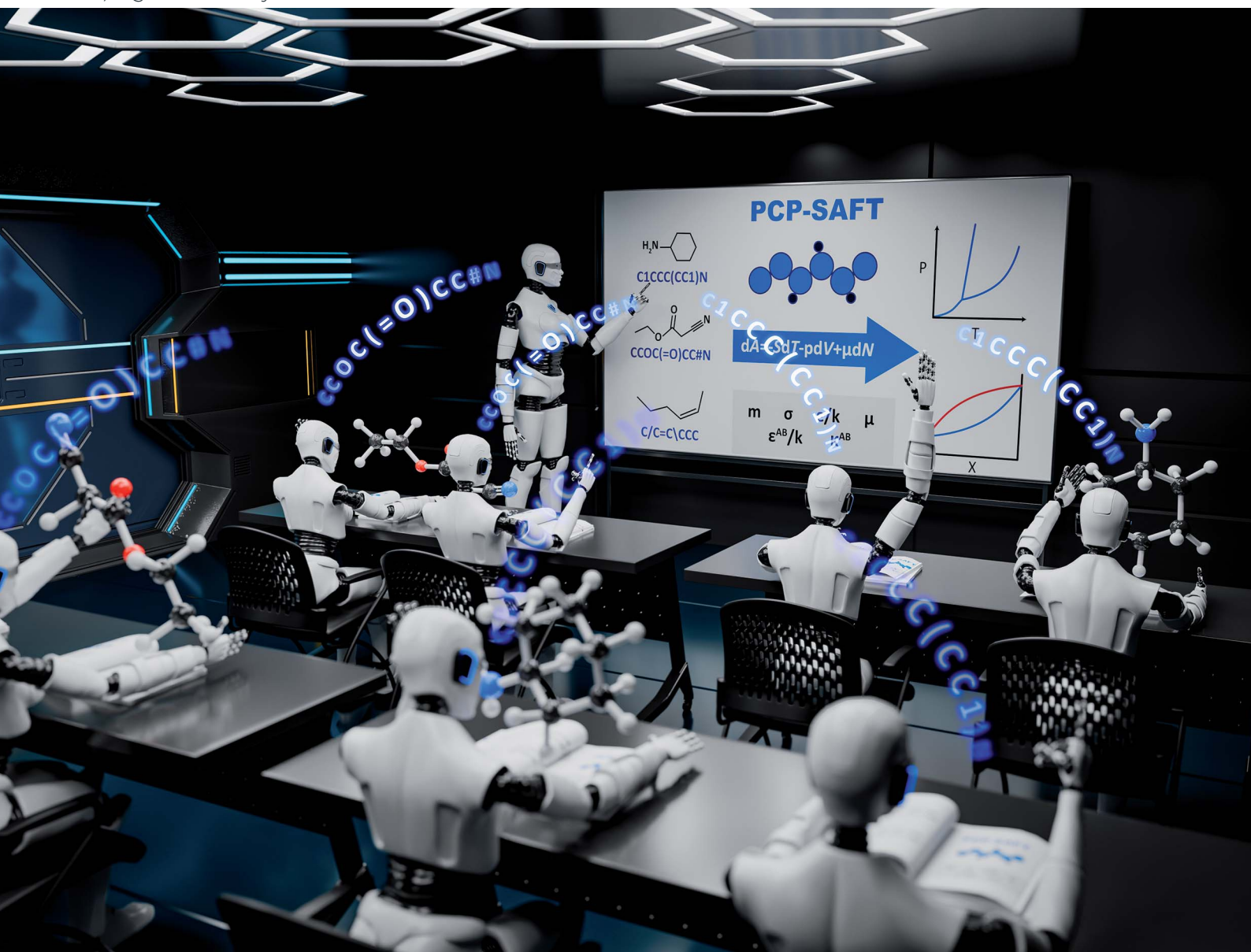


Digital Discovery

Volume 4
Number 5
May 2025
Pages 1115-1374

rsc.li/digitaldiscovery



ISSN 2635-098X

PAPER

André Bardow *et al.*

Understanding the language of molecules: predicting pure component parameters for the PC-SAFT equation of state from SMILES