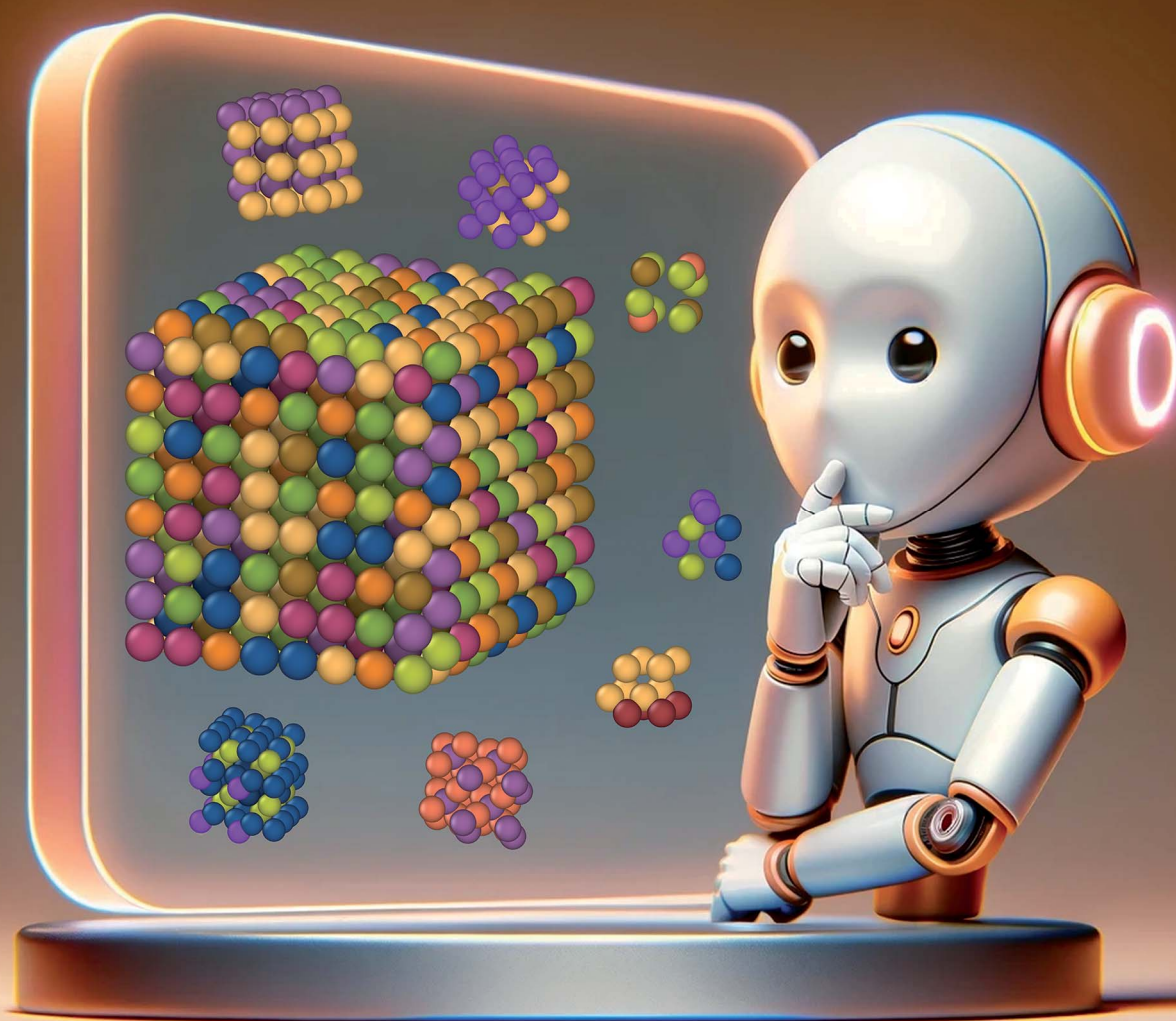


# Journal of Materials Chemistry A

Materials for energy and sustainability

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**PAPER**

Kangming Li, Jason Hatrick-Simpers *et al.*  
Efficient first principles based modeling *via* machine  
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