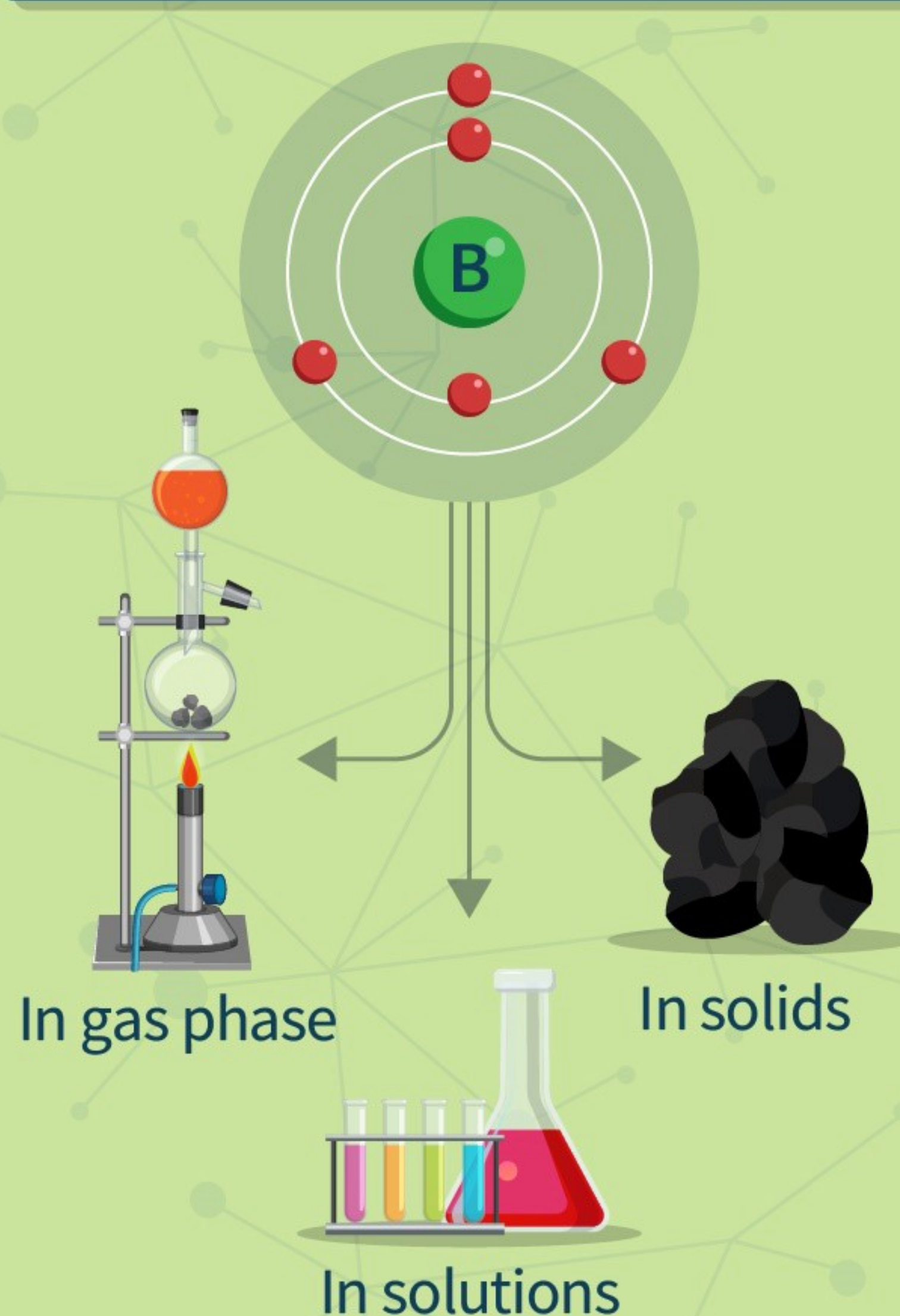


# Bridging Parallel Concepts in Boron Chemistry to Predict New Molecules and Materials

Chemical  
Science

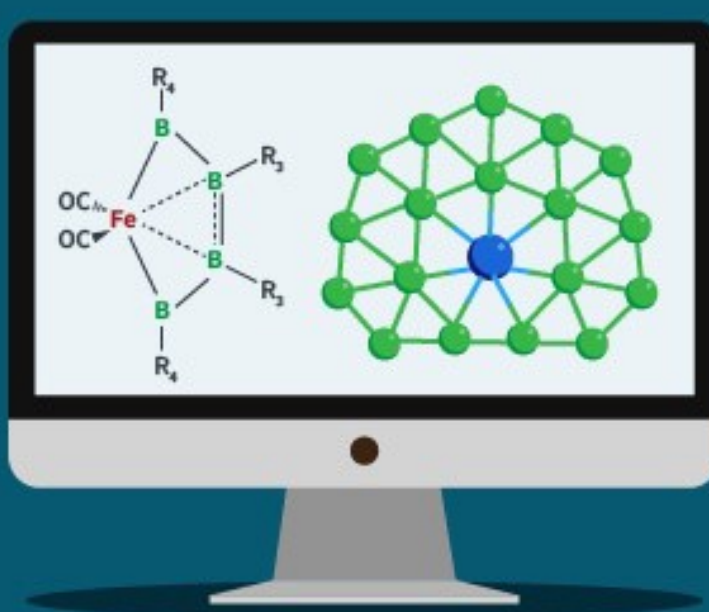
Boron chemistry has progressed immensely over the past few years, but it has done so in seemingly unrelated areas



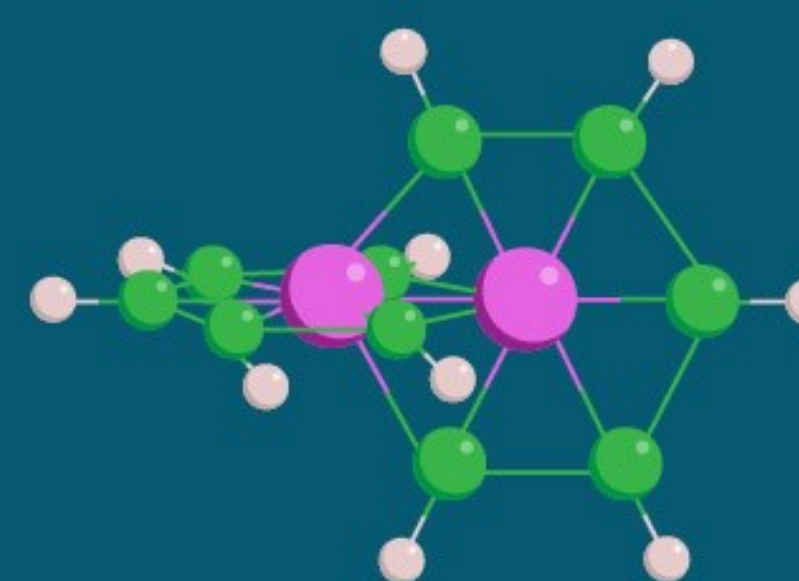
How can we discover and benefit from the interrelationships between them?

Finding a continuum between parallel fields in boron chemistry using density functional theory

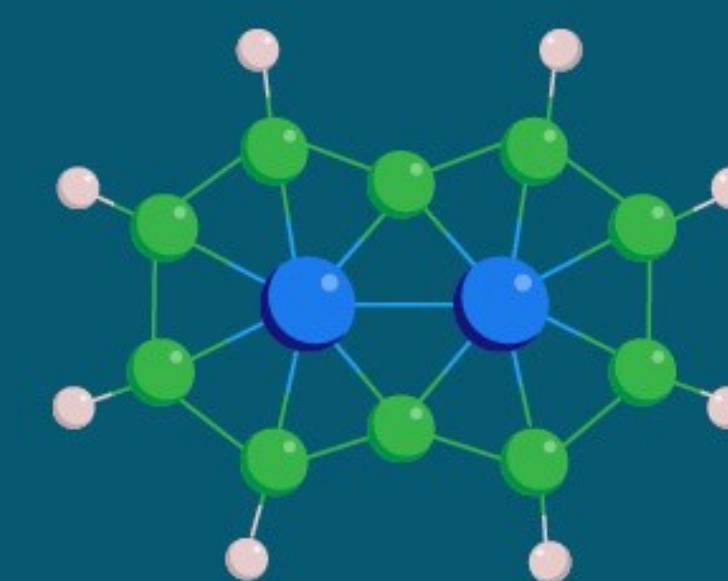
From molecules...



Analysis of B–B coupling (gas phase / in solution)

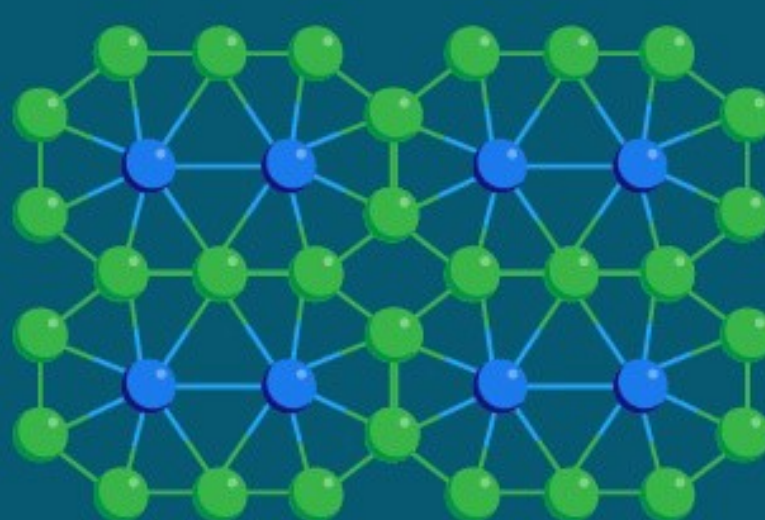


Interlocked boron wheel with Möbius aromaticity  
 $Mn_2B_{10}H_{10}$



Metal-doped boranaphthalene with Hückel aromaticity  
 $M_2@B_{10}H_8$  (M = Mn and Fe)

...to materials



2D sheets  
 $M_2B_5$

Results bridge molecular boron chemistry with the solid state by focusing on converging points



This strategy paves the way to further research into the hidden continuums between different areas of chemistry