

# RSC Applied Interfaces

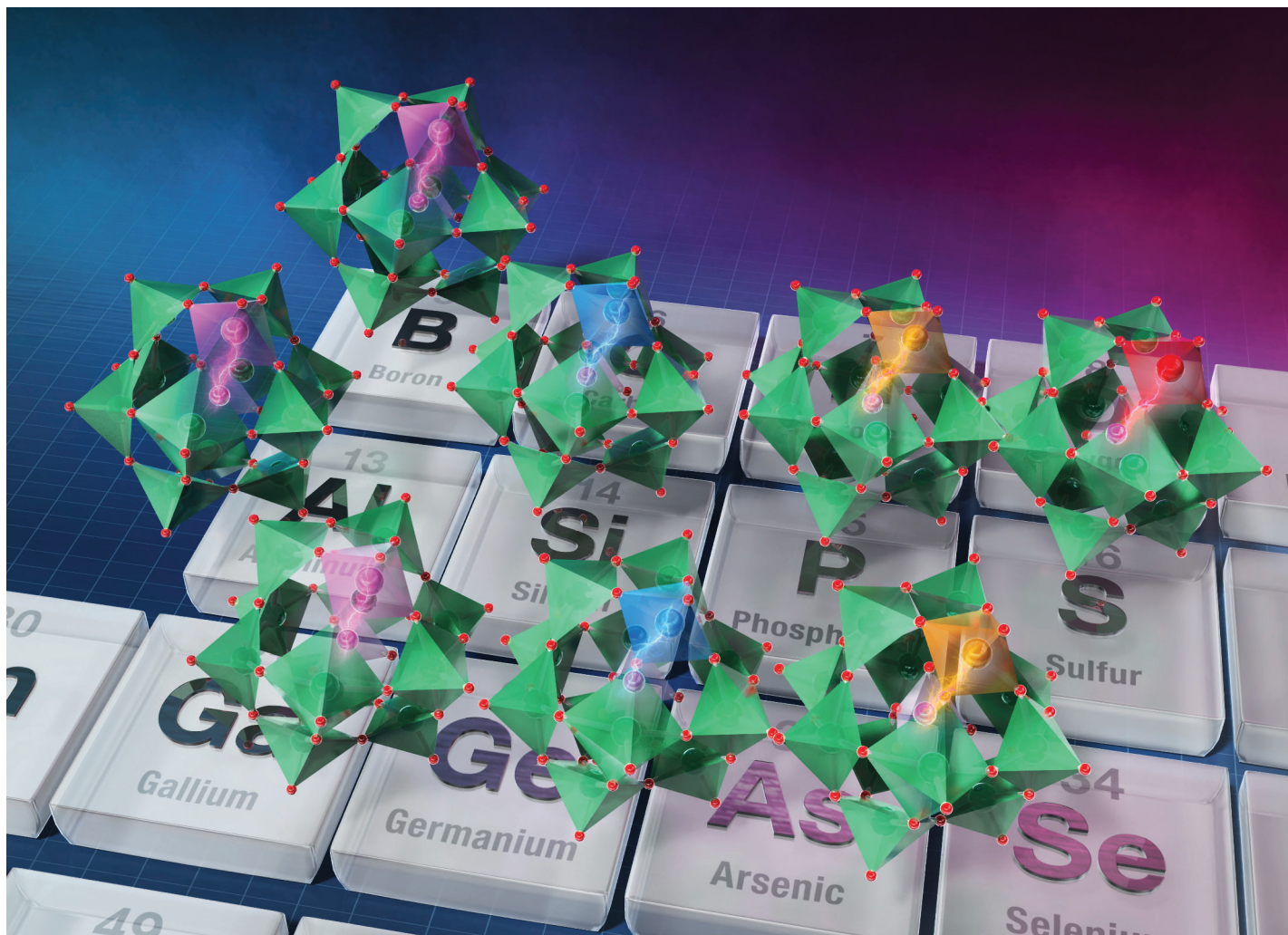
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**Interfacial and surface research  
with an applied focus**

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**Fundamental questions  
Elemental answers**



Showcasing research from Professor Sekine's laboratory,  
Waseda University, Tokyo, Japan.

Factors governing the protonation of Keggin-type  
polyoxometalates: influence of the core structure in clusters

In Keggin-type POMs, the first protonated position and energy were evaluated by DFT calculation, and these were governed by the addenda metal species, total charge, and the  $O_n-M$  bond length. The chemical and physical properties of the  $\beta$ -isomers could be predicted from the parameters of the  $\alpha$ -isomers.

As featured in:



See Yasushi Sekine *et al.*,  
*Dalton Trans.*, 2024, **53**, 8576.