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Computational cluster chemistry: from growth to catalysis

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Endohedral clusters, structures where one or more transition metal is encapsulated inside a shell of main-group atoms, present a perhaps uniquely diverse platform for exploring the nature of the chemical bond. Whilst the interactions between the metal and the cage can be, and indeed very often are, strong, radial bonding is not essential to the integrity of the structure. In this talk, I will focus on the rapidly expanding group of endohedral clusters that contain transition metals with incomplete *d* shells, and show how the complex interplay of metal-metal and metal-cage bonding leads to remarkable structural chemistry and spectroscopy. Both density functional theory and CASSCF methodologies are important tools in this regard, and I will discuss the merits of both techniques. I will also discuss spectroscopic and computational evidence that supports the idea that metal ions can act as a locus for cluster growth, and also how clusters might act as effective catalysts.

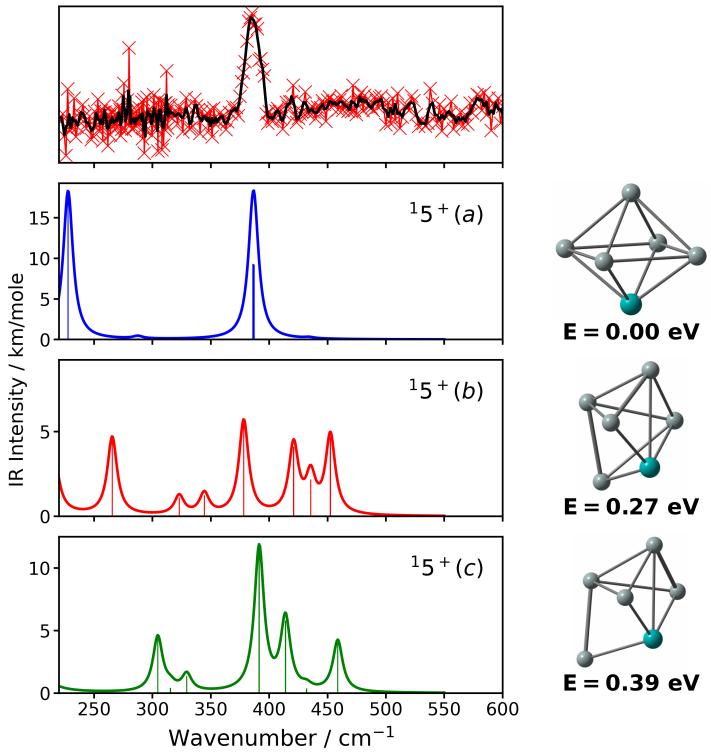

Figure 1 Vibrational spectroscopy of $[ReSi_5]^+$

1 **Electronic structure and bonding in endohedral Zintl clusters** J. E. McGrady, F. Weigend and S. Dehnen, *Chem. Soc. Rev.*, **2022**, *51*, 628.