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Interplay of geometric and electronic structure in metalloid gallium clusters DMITRI SCHEBARCHOV, NICOLA GASTON, Industrial Research Ltd. — Over the last two decades, the so-called "renaissance of main group chemistry" has led to significant advances in the synthesis, isolation and characterization of metalloid gallium clusters. What distinguishes these from other metalloid species (e.g. ligand-protected gold, silver, palladium, etc.) is their structural diversity, with the existence of four different Ga_{22} frameworks being a particularly striking example. To gain more insight into this polymorphism, we carried out electronic structure calculations using density functional theory. Our calculations verify that two of the ligand-protected Ga_{22} isomers can to some degree be viewed as superatom complexes - their respective metalloid cores are more or less close-packed, roughly spherical, and exhibit a well-defined electronic shell structure with a completely filled outer-most shell. The other two frameworks contain a slightly distorted icosahedral Ga_{12} core without a central atom - an unusual arrangement for metals - and the underlying electronic structure is more complex. This talk will serve as a summary of our calculations and illustrate the interplay of geometric and electronic structure in metalloid gallium clusters.

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