Remarkable Mixture of Germanium with Phosphorus and Arsenic Atoms Making Stable Pentagonal Hetero-Prisms $[\text{M@Ge}_5\text{E}_5]^+$, $\text{E} = \text{P, As}$ and $\text{M} = \text{Fe, Ru, Os}$

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Figure S1. Shapes, and relative energies (in kcal/mol) of the lower-lying isomer of FeGe$_5$P$_5^+$ cluster. The geometry optimizations and energy calculations were performed using B3P86 functional with 6-311+G(d) basis set for Ge, P and aug-cc-pVTZ basis for Fe.
Figure S2. Shapes, and relative energies (in kcal/mol) of the lower-lying isomer of RuGe₅P₅⁺ cluster. The geometry optimizations and energy calculations were performed using B3P86 functional with 6-311+G(d) basis set for Ge,P and aug-cc-pVTZ-PP basis set for Ru.
Figure S3. Shapes, and relative energies (in kcal/mol) of the lower-lying isomer of OsGe₅P₅⁺ cluster. The geometry optimizations and energy calculations were performed using B3P86 functional with 6-311+G(d) basis set for Ge,P and aug-cc-pVTZ-PP basis set for Os.
Figure S4. Shapes, and relative energies (in kcal/mol) of the lower-lying isomer of FeGe₅As₅⁺ cluster. The geometry optimizations and energy calculations were performed using B3P86 functional with 6-311+G(d) basis set for Ge,As and aug-cc-pVTZ basis set for Fe.
Figure S5. Shapes, and relative energies (in kcal/mol) of the lower-lying isomer of RuGe₅As₅⁺ cluster. The geometry optimizations and energy calculations were performed using B3P86 functional with 6-311+G(d) basis set for Ge,As and aug-cc-pVTZ-PP basis set for Ru.
Figure S6. Shapes, and relative energies (in kcal/mol) of the lower-lying isomer of OsGe₅As₅⁺ cluster. The geometry optimizations and energy calculations were performed using B3P86 functional with 6-311+G(d) basis set for Ge,As and aug-cc-pVTZ basis set for Os.
Figure S7. The MO diagram containing 18 electrons of RuGe₅P₅⁺ structure.

Figure S8. The MO diagram containing 18 electrons of OsGe₅P₅⁺ structure.
Figure S9. The MO diagram containing 18 electrons of FeGe$_5$As$_5^+$ structure.

Figure S10. The MO diagram containing 18 electrons of RuGe$_5$As$_5^+$ structure.
Figure S11. The MO diagram containing 18 electrons of OsGe$_5$As$_5^+$ structure.