In their paper, Meloni and Gingerich reported on preliminary theoretical results by our group (Sec. 3 and Ref. 24). We want to add relevant information here (a) on the structure of the SnBi molecule, and (b) on our computed atomization energies for SnBi$_n$ ($n=1–3$).

Table I shows geometries optimized in density-functional calculations using the B3LYP functional$^2$ together with our large-core relativistic effective-core potentials (ECPs)$^3$ and corresponding $[4s4p3d2f]$ valence basis sets.$^1,3$ It is to be noted that SnBi$_2$ has $C_{2v}$ equilibrium structure which is lower in energy by $\sim$154 kJ/mol [as obtained in single-point coupled-cluster calculations with single and double excitations and perturbative account of triples (CCSD(T))] than the $D_{oh}$ geometry reported by Meloni and Gingerich.

Also shown in Table I are atomization energies with respect to gradually improve on the accuracy of the large-core ECP B3LYP values, we first replaced the large-core ECPs$^5$ and changed from B3LYP to CCSD$^6$ and beyond.$^7$ In a second step, we attempt to gradually improve on the accuracy of the large-core ECP B3LYP values, we first replaced the large-core ECPs$^5$ and changed from B3LYP to CCSD$^6$ and beyond.$^7$

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of this work have been done using the MOLPRO\textsuperscript{7} suite of programs.

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