Šob, Legut, and Friák Reply: The authors of the preceding Comment [1] question our conclusion that the stability of the simple cubic (sc) structure of α-Po is due to the relativistic mass-velocity and Darwin terms [2] and defend their previous finding that the origin of the stable sc structure is the spin-orbit (SO) interaction. Their original paper [3] utilized the generalized gradient approximation (GGA) for the exchange and correlation energy whereas we employed the local-density approximation (LDA).

First, it should be noted that the GGA does not provide a better agreement with experimental observations in every case. For example, in Fe_3Al it gives an incorrect ground state, in contrast to the LDA [4]. It is also common wisdom that the LDA is somewhat better for 4*d* and 5*d* metals as well as for many *sp* elements. According to our findings presented in [2], this is also the case for polonium. The equilibrium volume of sc Po found in our calculations within the LDA with SO interaction included (LDA + SO) [5] equals 37.15 Å^3 and agrees within 1% with the experimental value of 37.43 Å^3 [7]. The value obtained within GGA + SO approach is by 6% higher than the experimental value (see Table I in [2]). This is the reason why we based our calculations on LDA, which we considered more reliable in this case.

The authors of the preceding Comment [1] also performed the LDA calculations without and with SO interaction. Prior to discussing their conclusions in more detail, let us note that inclusion of SO interaction leads to the considerable increase of the equilibrium atomic volume (by 5% according to our findings), both within the LDA and GGA (see Table I in [2]). It is surprising that this volume effect is not mentioned either in the preceding Comment [1] or in the paper [3] that are supposed to document impropriety of our conclusions. Ref. [3], based on GGA, gives just one single value of the equilibrium atomic volume of sc Po, specifically 37.14 Å (presumably the authors mean 37.14 Å^3). However, is this the volume obtained from GGA calculation without the SO interaction or for the GGA + SO case? Strangely enough, their value is nearly identical to that obtained in our LDA + SO calculation, 37.15 Å^3. This is very confusing. If the authors inadvertently reported the LDA + SO value of the equilibrium volume together with the GGA results, they should publish an Erratum as soon as possible to avoid any misunderstanding. Moreover, they should also clarify how the volume effect was included. The above mentioned ambiguities impair considerably the reliability of the results presented in [3], which are at the same time to document that our conclusions [2] are erroneous.

Notwithstanding, assuming that the volume change associated with the SO interaction has been correctly taken into account in [1,3], the preceding Comment [1] confirms our result that within the LDA (which describes the energetics of Po better than GGA), both calculations with and without the SO interaction give the sc structure of α-Po as the most stable [2]. Hence, the SO interaction cannot be regarded as providing the stabilization of the sc structure in α-Po. On the other hand, the mass-velocity and Darwin terms do stabilize the sc structure in α-Po [2] and the preceding Comment [1] does not disprove this conclusion.

Naturally, we can always ask whether there can be any other stabilizing agent. In principle, we are looking for an effect which, when omitted, would change the sign in the energy difference between the Te-like structure and sc structure. In [2], we demonstrated that such an agent is the mass-velocity and Darwin term. In the preceding Comment [1], the authors found that SO interaction also leads to this effect, but only if it is considered *solely* for the 6*s* and 6*p* states. In this sense, both conclusions might be regarded as correct. However, the energy difference between the sc and Te-like structures in the SR-5dSO case (i.e., with the SO interaction neglected only for 6*p* and 6*s* electrons) is merely 1.7 meV/atom [1] so this effect is not that strong. On the other hand, if the mass-velocity and Darwin terms are turned off this difference amounts to 0.3 mRy/atom [2], i.e., to 4 meV/atom. Hence, the effect of the mass velocity and Darwin term is more than twice as large as the effect of SO interaction for 6*p* and 6*s* states.

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