Phonon softening and superconductivity triggered by spin-orbit coupling in simple-cubic α-polonium crystals

Chang-Jong Kang, Kyoo Kim, and B. I. Min
Department of Physics, PCTP, Pohang University of Science and Technology, Pohang 790-784, Korea
(Received 16 December 2011; revised manuscript received 2 August 2012; published 20 August 2012)

We have investigated the mechanism of stabilizing the simple-cubic (sc) structure in polonium (α-Po), based on the phonon dispersion calculations using the first-principles all-electron band method. We have demonstrated that the stable sc structure results from the suppression of the Peierls instability due to the strong spin-orbit coupling (SOC) in α-Po. We have also discussed the structural chirality realized in β-Po, as a consequence of the phonon instability. Further, we have explored the possible superconductivity in α-Po, and predicted that it becomes a superconductor with $T_c \sim 4$ K. The transverse soft phonon mode at $\mathbf{q} \approx \frac{2}{3}$R, which is greatly influenced by the SOC, plays an important role both in the structural stability and the superconductivity in α-Po.

DOI: 10.1103/PhysRevB.86.054115 PACS number(s): 74.25.Kc, 61.50.Ks, 63.20.dk, 74.10.+v

I. INTRODUCTION

Polonium (Po), which belongs to chalcogen group in the periodic table, is unique in that it crystallizes in the simple-cubic (sc) structure.[1] Po having atomic number $Z = 84$ was discovered by Marie and Pierre Curie in 1898. Po exists in two metallic allotropes, α and β-Po. It is α-Po that has a sc structure. Above 348 K, α-Po transforms to β-Po, which has the trigonal structure.[2] Selenium (Se) and tellurium (Te), which are isoelectronic elements to Po in the chalcogen group, also have the trigonal spiral structure.[3] Note that the trigonal structure can be derived from the sc structure by elongation or contraction along the [111] direction,[4] which is known to occur due to the Peierls distortion in p-bonded systems of Se and Te.[5]

Recently, there have been several reports to explore the origin of the stabilized sc structure in Po.[6–11] The general consensus so far is that the large relativistic effects in Po play an important role. The Peierls instability tends to be suppressed in Po by the relativistic effects. However, there was controversy on the role of spin-orbit coupling (SOC) of $6p$ electrons. Min *et al.*[6] claimed that the SOC in addition to the scalar-relativistic (SR) effects of mass velocity and Darwin terms is essential, while Legut and co-workers[7,9] claimed that the SR effects are already enough to stabilize sc-Po. The refined and comprehensive band calculations by the former group, by considering all the relativistic corrections and different exchange-correlation functionals, show that the SOC of $6p$ states is really important in stabilizing the sc phase of Po.[8]

In general, the structural transition is induced by the phonon softening instability, and so the phonon dispersion calculations would provide evidence of the structural stability. Verstraete[11] calculated the phonon dispersion of sc-Po based on the pseudopotential band method, and showed that the phonon softening instability does not occur even without including the SOC. This result seems to support Legut *et al.*'s claim[7] that the SR terms are sufficient to stabilize the sc phase. Thereafter, a couple of other studies were reported on the phonon dispersion of the α-Po at the ambient pressure[12] and under the pressure,[13] by using the pseudopotential band method. Since Po has a tiny energy difference, order of 1 meV, between the sc and trigonal structures,[8] special caution is needed to calculate and analyze the phonon dispersions.

The structural energetics in Po is known to be very sensitive to the volume and the utilized exchange-correlation method in the band calculation.[8,10] The lattice constant a_{expt} of α-Po was first measured by Beamer *et al.*[14] to be 3.345 Å. Later, Desando *et al.*[15] reported the refined lattice constant of α-Po to be 3.359 Å. In the above band and phonon dispersion calculations, the old $a_{\text{expt}}^{\text{old}} = 3.345$ Å was referenced. In the present study, we have taken $a_{\text{expt}} = 3.359$ Å as a reference. We have found that the small difference in a_{expt} is important in analyzing the structural stability.

As mentioned above, the Peierls instability is the key physics in Po.[6,10–12] Even if the Peierls instability is suppressed by the SOC, α-Po in the sc phase would still have the soft phonon mode and so the strong electron-phonon (EP) coupling. Then the natural question is whether or not α-Po would have superconductivity. To our knowledge, superconductivity in Po has not been explored yet, probably due to its radioactive and toxic nature.

In this paper, we have investigated phonon and superconducting properties of α-Po, employing the first-principles all-electron band methods. The phonon dispersions and superconducting properties of α-Po are studied with and without the SOC at different volumes. By means of the phonon dispersion calculations, we have explicitly demonstrated that the stability of the sc phase arises from the SOC, which concludes the long-standing dispute on the origin of stable sc structure of Po. Further, we have predicted that α-Po is a superconductor with T_c of ~4 K.

II. COMPUTATIONAL DETAILS

We have employed the FLAPW band method,[16] implemented in the ELK package.[17] The Brillouin-zone integration has been carried out with a (24 × 24 × 24) **k**-point mesh, and $R_{\text{MT}}K_{\text{max}} = 9$ is employed. The SOC was included in the second-variational scheme and the local-density approximation (LDA) was used for the exchange-correlation energy. Actually, the choice of the LDA is a more stringent test for the phonon stability than that of the generalized gradient approximation (GGA), because the GGA always gives more softened phonons than the LDA. For sc-Po, $a_{\text{th}}^0 = 3.335$ Å

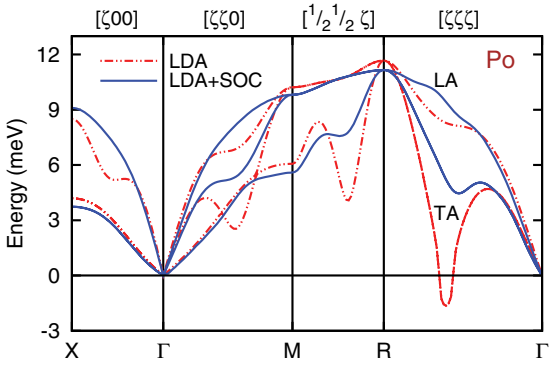

FIG. 1. (Color online) Phonon dispersions of sc-Po at $a = a_{\text{expt}}$ with SOC (LDA + SOC: blue solid line) and without it (LDA: red dotted line). The imaginary phonon frequencies are represented as negative values in the figure.

was obtained in the LDA + SOC scheme, which is in good agreement with $a_{\text{expt}} = 3.359$ Å of α-Po.

Phonon dispersions were obtained by using the supercell method, implemented in the ELK package. For phonon calculations, we have used the $(6 \times 6 \times 6)$ supercell, which describes softening behaviors in Po well. The force constants and the dynamical matrix are obtained from the Hellmann-Feynman forces calculated with small individual displacements of nonequivalent atoms.[18]

III. STABILITY OF SIMPLE-CUBIC STRUCTURE

Figure 1 shows the phonon dispersions of α-Po at $a = a_{\text{expt}}$ with and without the SOC. In the LDA scheme without the SOC (corresponding to the SR band scheme), the phonon softenings occur along all the high-symmetry directions. Among those, phonon frequency along Γ-R ($\mathbf{q} \approx \frac{2}{3}$R) is imaginary, which indicates the structural distortion along the [111] direction.[19] In contrast, in the LDA + SOC scheme (corresponding to the fully relativistic band scheme), the phonons become hardened and the imaginary phonon softening disappears. These features reflect that, without the $6p$ SOC, the sc structure of α-Po is unstable to a trigonal structure, as in Se and Te.

Note that, for the softened phonon at $\mathbf{q} \approx \frac{2}{3}$R, there are two degenerate normal modes having opposite helicities. The one has a clockwise helicity as shown in Fig. 2(b), while the other has a counterclockwise helicity. Thus the softened phonon at $\mathbf{q} \approx \frac{2}{3}$R induces the structural transformation to the trigonal β-Po, which has the helical chain structure with definite chirality [Fig. 2(c)]. The chiral structure realized in β-Po was once proposed in Te,[20] which was recently explained in terms of the orbital-ordered chiral charge-density wave (CDW).[21,22] This orbital-ordered CDW would be suppressed if the SOC were larger, as will be discussed in Fig. 3. The chirality of similar feature was also observed in $1T$-$TiSe_2$.[23] Interestingly, both Te and $1T$-$TiSe_2$ exhibit superconductivity under high pressure[24,25] and Cu intercalation,[26] respectively, suggesting that the superconductivity emerges when the CDW is suppressed.

The phonon softening in Fig. 1 is closely related to the Peierls mechanism. The phonon softening is described by the

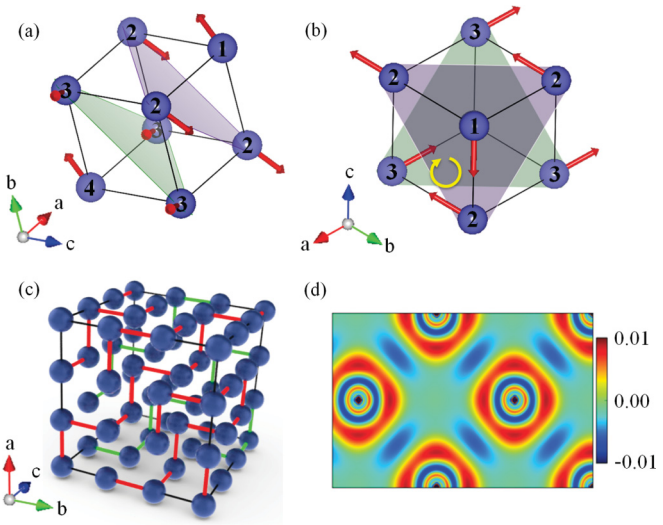

FIG. 2. (Color online) (a) One of two degenerate normal modes at $\mathbf{q} \approx \frac{2}{3}$R in sc-Po. All the displacement vectors are placed on (111) planes. (b) The same normal mode shown along the [111] viewpoint, which manifests a clockwise helicity. (c) The helical chain structure of β-Po with definite chirality. Red and green lines represent short bonds. (d) The difference of charge density of sc-Po in the LDA + SOC and that in the LDA (in units of $e/\text{Å}^3$). Notice the charge density depletion between neighboring ions.

renormalization of phonon frequency by the EP interaction (the so-called Kohn anomaly),

$$\omega^2(\mathbf{q}) = \Omega^2(\mathbf{q}) - |\tilde{g}_{\text{ep}}(\mathbf{q})|^2 \chi_0(\mathbf{q}), \tag{1}$$

where $\omega(\mathbf{q})$ and $\Omega(\mathbf{q})$ correspond to renormalized and bare phonon frequencies, respectively, and $\tilde{g}_{\text{ep}}$ and $\chi_0(\mathbf{q})$ are the EP coupling parameter and the charge susceptibility. Min *et al.*[6] obtained that $\chi_0(\mathbf{q})$ in α-Po has the highest peak at $\mathbf{q} \approx \frac{2}{3}$R due to the Fermi-surface nesting. They also showed that the SOC suppresses the Fermi-surface nesting effect and accordingly the $\chi_0(\mathbf{q})$ value, whereby they predicted that the phonon softening is weakened and finally the imaginary phonon softening disappears.

The suppression of the Peierls instability by the SOC occurs not only through the mechanism of Eq. (1) but also through

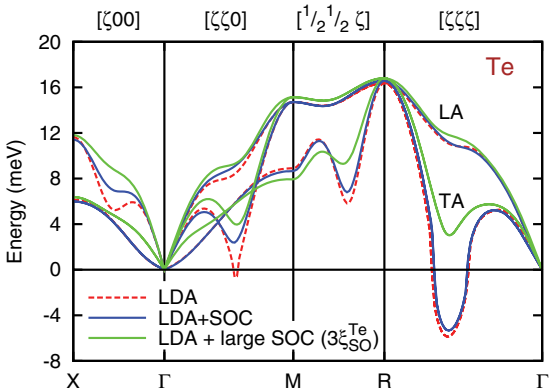

FIG. 3. (Color online) Phonon dispersion curves of sc-Te at the lattice constant of 3.210 Å, without the SOC (LDA), with the SOC (LDA + SOC), and with the three times larger SOC ($3\xi^{\text{Te}}_{\text{SO}}$).

weakening of the bonding strength. This feature is shown clearly in Fig. 2(d), which plots the difference of the charge density in the LDA + SOC and that in the LDA. It is evident that, due to the SOC, the charge density is depleted between the neighboring ions, which results in the weakening of the directional bondings of Po chains.

To verify the role of SOC in the structural stability more convincingly, we have examined the phonon dispersions of Te in the hypothetical sc structure (sc-Te) with artificially varying the strength of SOC of Te (ξ_{SO}^{Te}). Figure 3 shows that, in the LDA, two imaginary phonon softenings occur along the Γ-M and Γ-R directions, while, in the LDA + SOC, that remains only along the Γ-R direction. However, when we increase the SOC three times ($3\xi_{SO}^{Te}$), even the last imaginary phonon softening disappears eventually. This feature reveals that Te would also have a sc structure, if the SOC of Te becomes larger. The situation of the three times larger SOC in Fig. 3 actually simulates the case in Po, since the SOC of $6p$ electrons in Po ($\xi_{SO}^{Po} = 1.90$ eV) is almost three times stronger than that of $5p$ electrons in Te ($\xi_{SO}^{Te} = 0.72$ eV). The behavior in Fig. 3 provides definite evidence that the SOC really plays a role of suppressing the Peierls instability.

At the reduced volume, phonons tend to be hardened, and so it is expected that the phonon softening observed in Fig. 1 would be reduced. Indeed, the phonon dispersions of sc-Po at $a = 3.277$ Å ($V/V_{expt} = 0.93$) in Fig. 4(a) do not exhibit the imaginary phonon softenings both in the LDA and LDA + SOC schemes. Figure 4(b) shows the behavior of the phonon mode at $\mathbf{q} \approx \frac{2}{3}$R as a function of the lattice constant. It is seen that, with decreasing the lattice constant, the phonon frequency rises very steeply in the vicinity of a_{expt} (shaded area), and so the imaginary phonon softening disappears for $a < a_{expt}$. This is the reason why the phonon softening instability does not occur at $a_{th}^0 = 3.335$ Å ($V/V_{expt} = 0.98$) of the LDA + SOC, as in Verstraete's work,[11] but occurs at $a_{th}^0 = 3.411$ Å ($V/V_{expt} = 1.05$) of the GGA + SOC.[6] Moreover, since the α to β transformation in Po occurs at 348 K, one might have to take into account the thermal expansion (α_T) of the lattice constant.[28,29] Considering $\alpha_T = 23.5$ μm/m K of α-Po at 298 K,[27] the lattice elongation amounts to ~0.02 Å at 300 K, which is large enough to influence the phonon softening instability. In fact, the lattice constant of α-Po at 298 K is reported to be 3.366 Å ($V/V_{expt} = 1.01$).[27] Then, without the SOC, α-Po would be unstable to β-Po, as indicated by the filled blue square in Fig. 4(b).

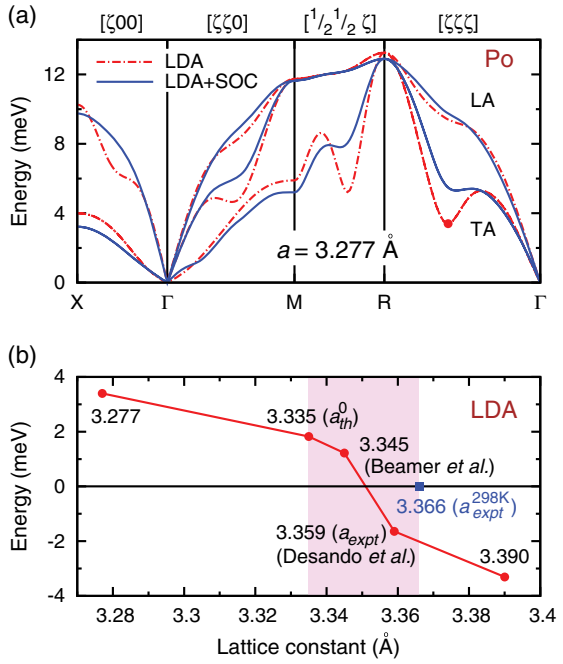

FIG. 4. (Color online) (a) The phonon dispersion curves of the sc-Po with and without the SOC at the reduced volume $V/V_{expt} = 0.93$ ($a = 3.277$ Å). The filled circle corresponds to the phonon mode at $\mathbf{q} \approx \frac{2}{3}$R. The overall phonon modes are hardened at the reduced volume. (b) The behavior of softened TA phonon mode at $\mathbf{q} \approx \frac{2}{3}$R in the LDA with varying the lattice constant. Here, $a = 3.335$ Å ($V/V_{expt} = 0.98$) corresponds to a_{th}^0 of the LDA + SOC, while $a = 3.345$ Å and $a = 3.359$ Å correspond to the low-temperature experimental lattice constants reported by Beamer *et al.* (Ref. 14) and by Desando *et al.* (Ref. 15), respectively. $a = 3.366$ Å (filled square) corresponds to the lattice constant at 298 K (Ref. 27).

IV. SUPERCONDUCTIVITY

We now consider the superconducting properties of the α-Po. α-Po has 33 known isotopes. Among those, the most abundant ^{210}Po has the half-life of 138.3 days, and the self-heating effect makes superconducting experiment difficult. On the other hand, ^{209}Po with a half-life of 103 years is less vulnerable to the self-heating effect, and so would be more pertinent to the superconducting experiment.

In the Eliashberg theory, the average EP coupling constant is given by

$$\lambda = 2\int_0^\infty d\omega \alpha^2 F(\omega)/\omega \tag{2}$$

with the Eliashberg function expressed as

$$\alpha^2 F(\omega) = \frac{1}{N(E_F)} \sum_{\mathbf{q}\nu} \sum_{\mathbf{k},n,m} \left| g_{\mathbf{k}n,\mathbf{k}+\mathbf{q}m}^{\nu} \right|^2 \times \delta(\epsilon_{\mathbf{k}n}) \delta(\epsilon_{\mathbf{k}+\mathbf{q}m}) \delta(\omega - \omega_{\mathbf{q}\nu}). \tag{3}$$

Here $N(E_F)$ is the DOS at E_F, and $\omega_{\mathbf{q}\nu}$ denotes the frequency of the phonon mode ν with momentum $\mathbf{q}$. The EP matrix element $g_{\mathbf{k}n,\mathbf{k}+\mathbf{q}m}^{\nu}$ is obtained from $g_{\mathbf{k}n,\mathbf{k}+\mathbf{q}m}^{\nu} = \langle \mathbf{k}n | \mathbf{e}_{\mathbf{q}\nu} \cdot \nabla V_{KS}(\mathbf{q}) | \mathbf{k}+\mathbf{q}m \rangle / \sqrt{2M\omega_{\mathbf{q}\nu}}$, where $\mathbf{e}_{\mathbf{q}\nu}$ is the polarization vector and $\nabla V_{KS}(\mathbf{q})$ is the gradient of the Kohn-Sham potential with respect to the atomic displacements with the wave vector $\mathbf{q}$. Then the critical temperature T_c is obtained with the McMillan-Allen-Dynes formula:[30]

$$T_c = \frac{\omega_{ln}}{1.20} \exp\left(-\frac{1.04(1+\lambda)}{\lambda - \mu^* - 0.62\lambda\mu^*} \right), \tag{4}$$

where $\omega_{ln}(\equiv \exp[\frac{2}{\lambda}\int_0^\infty \frac{d\omega}{\omega}\alpha^2 F(\omega)\ln\omega])$ is the logarithmic average frequency and μ^* is the effective Coulomb repulsion parameter. The estimated superconducting parameters are listed in Table I.

Noteworthy in Table I is that α-Po at the ambient pressure ($V/V_{expt} = 0.98$) would be a superconductor with $\lambda = 0.89$ and $T_c \sim 4$ K. At the reduced volume ($V/V_{expt} = 0.93$), both

TABLE I. DOS at E_F, $N(E_F)$, Debye temperature θ_D, and the superconducting parameters of α-Po. Two values of T_c are for two different values of $\mu^* = 0.10$ and 0.13.

	V/V_{expt}	$N(E_F)$ (states/eV)	θ_D (K)	λ	$\omega_{\ln}$ (meV)	T_c (K)
LDA+	1	0.63	103.7	0.76	6.66	3.38, 2.67
SOC	0.98	0.60	101.5	0.89	6.52	4.34, 3.78
	0.93	0.57	113.3	1.04	6.52	5.57, 5.10
LDA	0.98	0.61	102.5	0.95	6.43	5.04, 4.25
	0.93	0.57	110.6	1.11	6.69	6.28, 5.85

λ and T_c increase further to 1.04 and ~5 K, respectively. With reducing the volume, $N(E_F)$ decreases, while the Debye temperature θ_D increases. The effect of the SOC on the superconductivity is found to be not so large but detrimental. For $V/V_{\text{expt}} = 0.93$, the SOC reduces λ from 1.11 to 1.04, and T_c from ~6 K to ~5 K. It is mainly because of the phonon hardening induced by the SOC, as discussed in Figs. 1 and 4. This behavior in Po is quite opposite to that in neighboring element Pb, for which the SOC rather softens the phonons and increases λ by more than 40%.[31–33] This difference is thought to arise from the different Fermi-surface nature between the two.[31]

To examine which phonon contributes largely to superconductivity, we computed the **q**-dependent EP coupling constant $\lambda_{\mathbf{q}\nu}$. As shown in Figs. 5(a)–5(c), $\lambda_{\mathbf{q}\nu}$'s show peaks at **q**'s having phonon softening anomalies along Γ-X, M-R, and Γ-R directions. Longitudinal X and transverse Γ-R phonon modes have fairly large values of $\lambda_{\mathbf{q}\nu}$. We found above that λ in sc-Po increases as the volume is reduced. In view of the phonon hardening at reduced volume, this behavior looks strange, at first glance. The enhanced λ can be explained by the behavior of the Eliashberg function $\alpha^2F(\omega)$ in Figs. 5(d) and 5(e). At the reduced volume, the maximum cutoff frequency is larger, and $\alpha^2F(\omega)$ is enhanced at low frequency. This leads to enhanced λ and higher T_c. As shown in Figs. 5(d) and 5(e), the integrated Eliashberg function $\lambda(\omega)$ has a steep rise at about 4 and 5 meV for $V/V_{\text{expt}} = 0.98$ and $V/V_{\text{expt}} = 0.93$, respectively. This energy range corresponds to that of the transverse Γ-R soft phonon mode (Fig. 4), suggesting that the superconductivity of sc-Po comes largely from the $\mathbf{q} \approx \frac{2}{3}\mathrm{R}$ phonon mode. In the LDA scheme of Fig. 5(c), the $\mathbf{q} \approx \frac{2}{3}\mathrm{R}$ soft phonon mode produces the larger $\lambda_{\mathbf{q}\nu}$, while in the LDA + SOC scheme of Fig. 5(b), the $\mathbf{q} \approx \frac{2}{3}\mathrm{R}$ phonon mode hardened by the SOC reduces $\lambda_{\mathbf{q}\nu}$ by half. This is the reason why the SOC is detrimental to the superconductivity in Po.

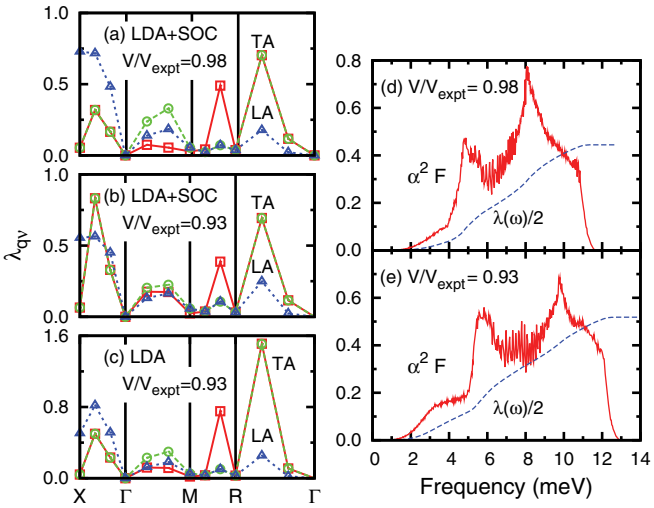

FIG. 5. (Color online) The **q**-dependent EP coupling constants of α-Po: (a) in the LDA + SOC for $V/V_{\text{eq}} = 0.98$, (b) in the LDA + SOC for $V/V_{\text{eq}} = 0.93$, (c) in the LDA for $V/V_{\text{eq}} = 0.93$. The Eliashberg functions $\alpha^2F(\omega)$ with the SOC at different volumes of α-Po: (d) in the LDA + SOC for $V/V_{\text{eq}} = 0.98$, (e) in the LDA + SOC for $V/V_{\text{eq}} = 0.93$. Integrated Eliashberg functions $\lambda(\omega)$ are shown.

V. CONCLUSION

Based on the phonon dispersion calculations, we have explicitly demonstrated that the SOC is the origin of the stabilized sc structure of α-Po. The SOC suppresses the phonon softening instability at $\mathbf{q} \approx \frac{2}{3}\mathrm{R}$, which, otherwise, would induce the structural transformation to trigonal β-Po. We have also predicted that α-Po would be a superconductor with $T_c \sim 4$ K. The soft transverse phonon modes at $\mathbf{q} \approx \frac{2}{3}\mathrm{R}$ in α-Po, which are greatly influenced by the SOC, play an important role both in the structural stability of the sc phase and its superconductivity. The experimental verification of the superconductivity in α-Po is demanded.

ACKNOWLEDGMENTS

This work was supported by the NRF (Grants No. 2009-0079947 and No. 2011-0025237) and the KISTI supercomputing center (Grants No. KSC-2011-C2-36 and No. KSC-2012-C3-09).

[1] W. H. Beamer and C. R. Maxwell, J. Chem. Phys. **14**, 569 (1946).
[2] C. R. Maxwell, J. Chem. Phys. **17**, 1288 (1949).
[3] H. J. Beister, K. Strössner, and K. Syassen, Phys. Rev. B **41**, 5535 (1990).
[4] G. Kresse, J. Furthmuller, and J. Hafner, Phys. Rev. B **50**, 13181 (1994).
[5] J. K. Burdett and S. Lee, J. Am. Chem. Soc. **105**, 1079 (1983).
[6] B. I. Min, J. H. Shim, M. S. Park, Kyoo Kim, S. K. Kwon, and S. J. Youn, Phys. Rev. B **73**, 132102 (2006).
[7] D. Legut, M. Friák, and M. Šob, Phys. Rev. Lett. **99**, 016402 (2007).
[8] K. Kim, H. C. Choi, and B. I. Min, Phys. Rev. Lett. **102**, 079701 (2009).
[9] M. Šob, D. Legut, and M. Friák, Phys. Rev. Lett. **102**, 079702 (2009).
[10] D. Legut, M. Friák, and M. Šob, Phys. Rev. B **81**, 214118 (2010).
[11] M. J. Verstraete, Phys. Rev. Lett. **104**, 035501 (2010).
[12] A. Belabbes, A. Zaoui, and M. Ferhat, Solid State Commun. **150**, 2337 (2010).

[13] A. Zaoui, A. Belabbes, R. Ahuja, and M. Ferhat, Phys. Lett. A **375**, 1695 (2011).
[14] W. H. Beamer and C. R. Maxwell, J. Chem. Phys. **17**, 1293 (1949).
[15] R. J. Desando and R. C. Lange, J. Inorg. Nucl. Chem. **28**, 1837 (1966).
[16] M. Weinert, E. Wimmer, and A. J. Freeman, Phys. Rev. B **26**, 4571 (1982).
[17] The Elk FP-LAPW Code; http://elk.sourceforge.net/.
[18] R. Yu, D. Singh, and H. Krakauer, Phys. Rev. B **43**, 6411 (1991); B. Kohler, S. Wilke, M. Scheffler, R. Kouba, and C. Ambrosch-Draxl, Comput. Phys. Commun. **94**, 31 (1996).
[19] When the GGA (PBE) and PBEsol schemes are used, phonons are more softened to produce two imaginary phonon softenings along the M-R and Γ-R directions, at both a_{expt} and a_{th}^{0} of the LDA + SOC.
[20] H. Fukutome, Prog. Theor. Phys. **71**, 1 (1984).
[21] J. van Wezel and P. Littlewood, Physics **3**, 87 (2010).
[22] J. van Wezel, Europhys. Lett. **96**, 67011 (2011).
[23] J. Ishioka, Y. H. Liu, K. Shimatake, T. Kurosawa, K. Ichimura, Y. Toda, M. Oda, and S. Tanda, Phys. Rev. Lett. **105**, 176401 (2010).
[24] Y. Akahama, M. Kobayashi, and H. Kawamura, Solid State Commun. **84**, 803 (1992).
[25] F. Mauri, O. Zakharov, S. de Gironcoli, S. G. Louie, and M. L. Cohen, Phys. Rev. Lett. **77**, 1151 (1996).
[26] E. Morosan, H. W. Zandbergen, B. S. Dennis, J. W. G. Bos, Y. Onose, T. Klimczuk, A. P. Ramirez, N. P. Ong, and R. J. Cava, Nat. Phys. **2**, 544 (2006).
[27] *CRC, Handbook of Chemistry and Physics*, 86th ed., edited by D. R. Lide (CRC, Boca Raton, FL, 2005).
[28] B. Grabowski, T. Hickel, and J. Neugebauer, Phys. Rev. B **76**, 024309 (2007).
[29] A. J. Hatt, B. C. Melot, and S. Narasimhan, Phys. Rev. B **82**, 134418 (2010).
[30] P. B. Allen and R. C. Dynes, Phys. Rev. B **12**, 905 (1975).
[31] M. J. Verstraete, M. Torrent, F. Jollet, G. Zérah, and X. Gonze, Phys. Rev. B **78**, 045119 (2008).
[32] A. Dal Corso, J. Phys.: Condens. Matter **20**, 445202 (2008).
[33] R. Heid, K.-P. Bohnen, I. Yu. Sklyadneva, and E. V. Chulkov, Phys. Rev. B **81**, 174527 (2010).