ERRATA

Erratum: Effect of zero-point corrections and *k*-point sampling on the structural stability determinations of alkali metals [Phys. Rev. B 54, 10 253 (1996)]

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Several statements should be included in this paper. We regret the omission of linear muffin-tin orbital–atomic sphere approximation calculations of Boettger and Albers[1] and the subsequent full-potential linear augmented plane wave work of Nobel *et al.*,[2] both of which found hcp to be the equilibrium phase for Li, in Table I. We should also have emphasized that the calculations of both Boettger and Trickey[3] and of Sigalas *et al.*[4] were restricted only to cubic symmetries, in order to avoid misleading the reader regarding Li and Na in Table I.

We should have stated that the treatment of Brillouin zone (BZ) scan sensitivity is not new, and we should have included a discussion of the references that have a bearing on this subject. Both Refs. 1 and 2 point out explicitly the sensitivity of the Li structural stability determination to BZ scans. The first detailed study of this sensitivity was presented in Dacorogna and Cohen's paper,[5] which was discussed in Ref. 2, and Ref. 1 noted that the problem had been mentioned in Ref. 3. It is also emphasized in Ref. 2 that the anomalous ground-state symmetry predicted for Li in Ref. 6 is a result of that sensitivity, which was rediscovered in Ref. 4.

We should also emphasize that highly converged full-potential local-density approximation (LDA) and generalized gradient approximation calculations[7,8] predict the ground state of K as fcc, in contradiction to experiment. A full-potential result is to be believed over an atomic sphere approximation result, and that this is contradictory with experiment should be considered as the fault of the LDA as emphasized in Ref. 7. This is confirmed by our previous calculations[9] in which nonlocal corrections to the LDA were included as proposed in Ref. 7. Therefore, in our opinion, it is desirable to invent a LDA representation that predicts the correct ground state of all metals when used with a full-potential method.

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[1] J. C. Boettger and R. C. Albers, Phys. Rev. B **39,** 3010 (1989).
[2] J. A. Nobel, S. B. Trickey, P. Blaha, and K. Schwarz, Phys. Rev. B **45,** 5012 (1992).
[3] J. C. Boettger and S. B. Trickey, Phys. Rev. B **32**, 3391 (1985).
[4] M. Sigalas, N. C. Bacalis, D. A. Papaconstantopoulos, M. J. Mehl, and A. C. Switendick, Phys. Rev. B **42,** 11 637 (1990).
[5] M. M. Dacorogna and M. L. Cohen, Phys. Rev. B **34,** 4996 (1986).
[6] M. Bross and R. Stryczek, Phys. Status Solidi B **144,** 675 (1987).
[7] D. A. Papaconstantopoulos and D. J. Singh, Phys. Rev. B **45,** 7507 (1992).
[8] S. B. Trickey, K. Schwarz, P. Blaha, and J. C. Boettger (unpublished).
[9] R. H. Mutlu, Phys. Rev. B **52,** 1441 (1995).

