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CORRECTION

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Correction: Solvation of Li^+ by argon: how important are three-body forces?

Frederico V. Prudente, [a] Jorge M. C. Marques [b] and Francisco B. Pereira [cd]

Correction for 'Solvation of Li^+ by argon: how important are three-body forces?' by Frederico V. Prudente *et al.*, *Phys. Chem. Chem. Phys.*, 2017, **19**, 25707–25716.

The authors detected an error in the code that implements eqn (8): the factor "3" multiplying C_9 was missing in the Fortran program of PES I. After correction, we have searched for the global minimum structures of Li^+Ar_n (n = 3–40) for the PES I with the evolutionary algorithm. The results lead to the following corrections in the paper:

(1) The table and figures below should replace Table 3, Fig. 3, Fig. 4, Fig. 5, Fig. 6, Fig. 7 and Fig. 8, respectively.

(2) On the bottom of the right column on page 25711, the sentence beginning as "The energy difference..." (first paragraph of Section 3.2) must be replaced by: "The energy difference between the two potentials increases from $\sim$1.2 mE_h ($\sim$6%) for n = 2 to $\sim$35.6 mE_h ($\sim$29%) for n = 40."

(3) On the bottom of the left column and on the top of the right column on page 25712 (*i.e.*, the end of the second paragraph of Section 3.2), the text should read: "Although most of the global minima are similar for the three potentials, it is worth noting that the outcome provided by PES I disagrees with the MP2 one for n = 9, whereas PES II shows different structures for n = 2, 3 and 10. In addition, we have also performed MP2 re-optimizations departing from the lowest-energy structures of PES II for n = 2, 3 and 9. The geometries so obtained for n = 2 and n = 3 are similar to those from PES I, which is a further indication of the importance of three-body interactions to reach structural accuracy of the global minima. In contrast for n = 9, departing from the global minimum geometry of either PES I or PES II, the MP2 re-optimization leads to different structures and the one corresponding to PES II has the lowest energy (*cf.* Fig. 3)."

(4) The two last sentences of the right column on page 25714 must be changed to read: "Moreover, Fig. 7 and Table 3 show that, besides the above-mentioned small clusters (namely for n = 1, 4–8), there are other larger clusters with identical structures for both PES I and PES II. Such structures arise in the size range $30 \leq n \leq 40$ and are depicted in Fig. 8."

(5) On the left column of page 25715, fourth and fifth sentences before the end of the first paragraph of Section 4 must be replaced by: "The Li^+Ar_n clusters obtained from PES I had a good agreement with the corresponding ones optimized at the *ab initio* level for n = 1–8 and 10. Although the PES II global minimum structure coincides with that from MP2 optimization for n = 9, this potential function leads to distinct geometries for Li^+Ar_2, Li^+Ar_3 and Li^+Ar_{10}, and fails to represent the main energetic features up to n = 10."

Although the energies of the global minima for PES I are, obviously, different from the values in the original paper, the corresponding geometries only vary for n = 9, 19, 20, 31 and 40 (see Table 3). For n = 9, the lowest-energy structure at the MP2 level of theory coincides with the global minimum for PES II (see Fig. 3); actually, the corresponding lowest-energy structure from the PES I is a local minimum at the MP2 level of theory. In turn, the average binding energy, the sublimation energy and the second difference in energy keep essentially the same pattern (see Fig. 4). Finally, we should emphasize that these results confirm the main conclusions of the paper about the importance of three-body interactions for the title system.

Ab initio energies and coordinates of all clusters in this work can now be found in the Electronic Supplementary Information file available alongside the original article.

[a] *Instituto de Física, Universidade Federal da Bahia, 40170-115 Salvador, BA, Brazil. E-mail: prudente@ufba.br*
[b] *CQC, Department of Chemistry, University of Coimbra, 3004-535 Coimbra, Portugal. E-mail: qtmarque@ci.uc.pt*
[c] *Instituto Superior de Engenharia de Coimbra Quinta da Nora, 3030-199 Coimbra, Portugal*
[d] *Centro de Informática e Sistemas da Universidade de Coimbra (CISUC), 3030-290 Coimbra, Portugal. E-mail: xico@dei.uc.pt*

Table 3 Energies (V_{GM}) and symmetries (SYM) of the putative global minima of Li^+Ar_n ($1 \leq n \leq 40$) obtained with the EA for both PES I and PES II; the RMSD values between the PES I and PES II structures are also indicated. Energies in mE_h and RMSD in a_0

	PES I		PES II		
n	V_{GM}	SYM	V_{GM}	SYM	RMSD
1	−10.6156	$C_{\infty v}$	−10.6156	$C_{\infty v}$	0.00
2	−20.4677	$D_{\infty h}$	−21.6866	C_{2v}	1.66
3	−29.3372	D_{3h}	−33.2131	C_{3v}	0.93
4	−37.1950	T_d	−45.1235	T_d	0.10
5	−42.2282	C_{4v}	−55.3408	C_{4v}	0.16
6	−47.4114	O_h	−66.3792	O_h	0.20
7	−49.2123	C_{3v}	−69.0324	C_{3v}	0.23
8	−51.0488	C_{2v}	−71.8400	C_{2v}	0.29
9	−52.8727	C_{3v}	−74.5812	C_s	2.36
10	−55.0185	C_s	−77.4174	C_{4v}	1.86
11	−57.1545	C_s	−80.1327	C_s	2.26
12	−59.2801	C_{3v}	−82.9402	C_{2v}	2.93
13	−61.5426	C_s	−85.7355	C_{3v}	2.79
14	−63.8410	C_{2v}	−88.6286	O_h	2.88
15	−66.0022	C_s	−91.2832	C_{3v}	2.44
16	−68.1649	C_{2v}	−94.1454	C_{3v}	2.66
17	−70.2635	C_s	−96.7194	C_s	2.60
18	−72.3542	C_{2v}	−99.6969	C_{2v}	2.70
19	−74.6213	C_s	−102.2157	C_s	2.89
20	−76.8875	C_s	−105.2226	C_{3v}	2.85
21	−79.0391	C_1	−107.7581	C_s	2.55
22	−81.2321	C_1	−110.6664	C_s	2.23
23	−83.6009	C_s	−113.2250	C_1	2.16
24	−85.9783	C_3	−116.1347	C_s	2.63
25	−88.4916	C_3	−118.7100	C_s	2.28
26	−90.5702	C_1	−121.6112	C_{3v}	2.12
27	−92.7125	C_1	−124.0709	C_1	2.36
28	−95.2238	C_3	−126.9316	C_2	2.72
29	−97.3301	C_1	−129.5222	C_1	2.63
30	−99.6171	D_{2d}	−132.4044	D_{2d}	0.24
31	−101.8398	C_1	−134.9826	C_s	2.07
32	−104.4660	C_2	−137.8239	C_{2v}	1.22
33	−106.6944	C_1	−140.4135	C_s	1.27
34	−109.3778	T	−143.4439	T	0.26
35	−111.6685	D_3	−146.0222	D_3	0.35
36	−113.6036	C_2	−148.2719	C_2	0.34
37	−116.0264	C_{3v}	−150.8371	C_{3v}	2.80
38	−118.8373	O_h	−154.1266	O_h	0.24
39	−120.8533	C_{4v}	−156.2772	C_{4v}	0.24
40	−122.8692	C_{2v}	−158.4278	C_{2v}	0.24

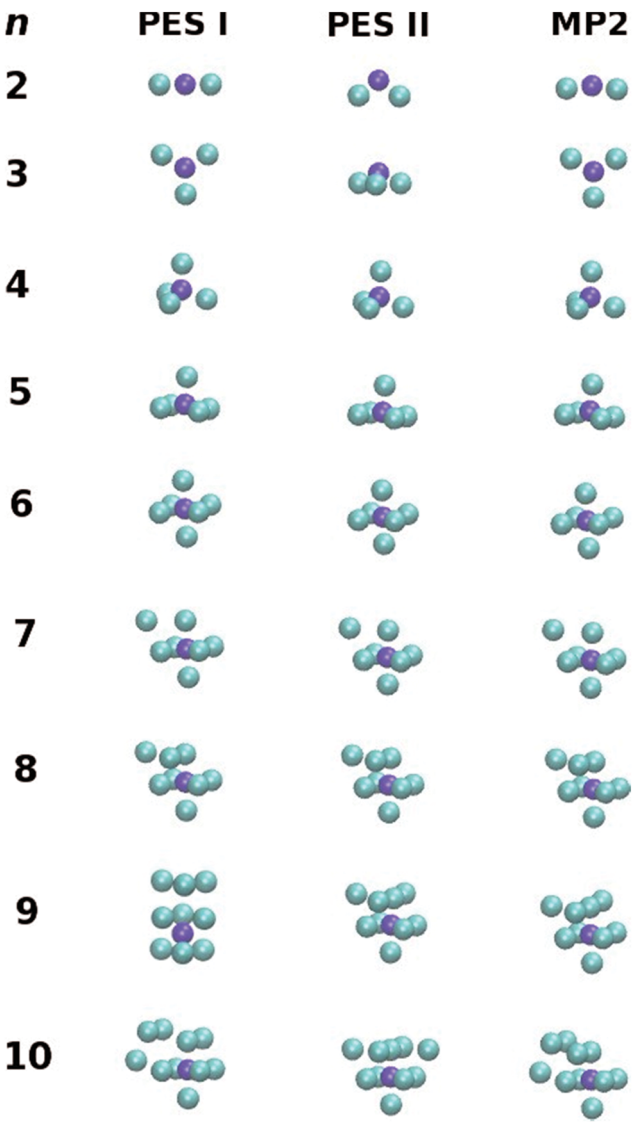

Fig. 3 Putative global minimum structures for PES I, PES II and MP2 up to n = 10.

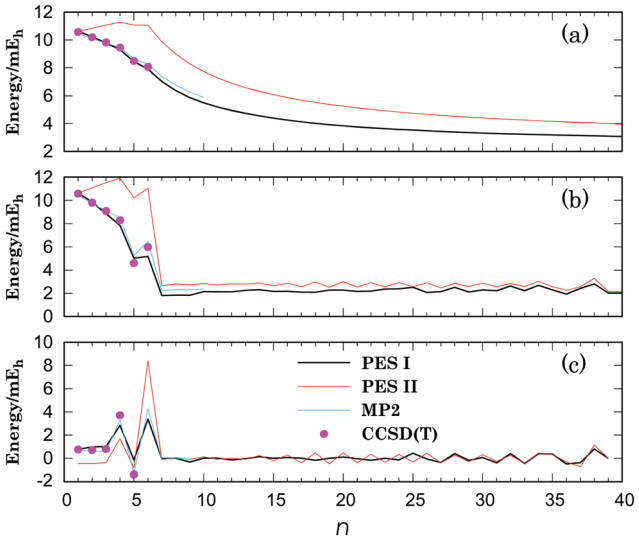

Fig. 4 Binding energy (a), sublimation energy (b) and second energy-difference (c) for Li^+Ar_n (n = 1–40) clusters. The key for symbols are in panel (c): PES I (black line); PES II (red line); MP2 optimization (light-blue line); CCSD(T) single-point calculation (magenta dots). Plotted values are obtained from the putative global minima at each level of theory.

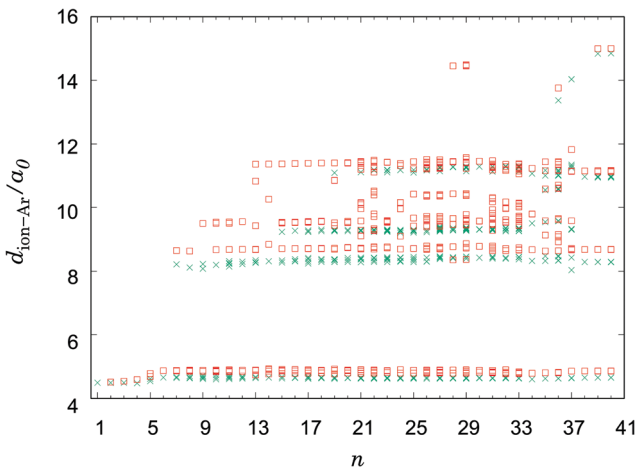

Fig. 5 Scatter plot of the distances between the Li^+-ion and the argon atoms: PES I (open squares); PES II (crosses).

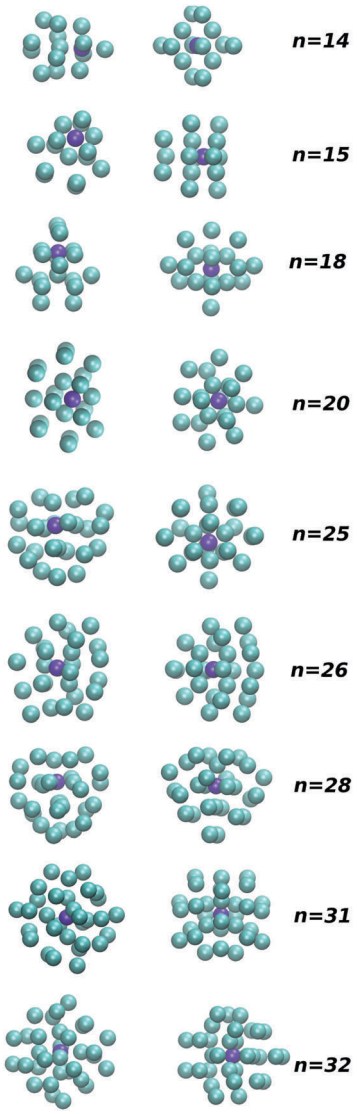

Fig. 6 Putative global minimum structures for PES I (left) and PES II (right) for n = 14, 15, 18, 20, 25, 26, 28, 31 and 32.

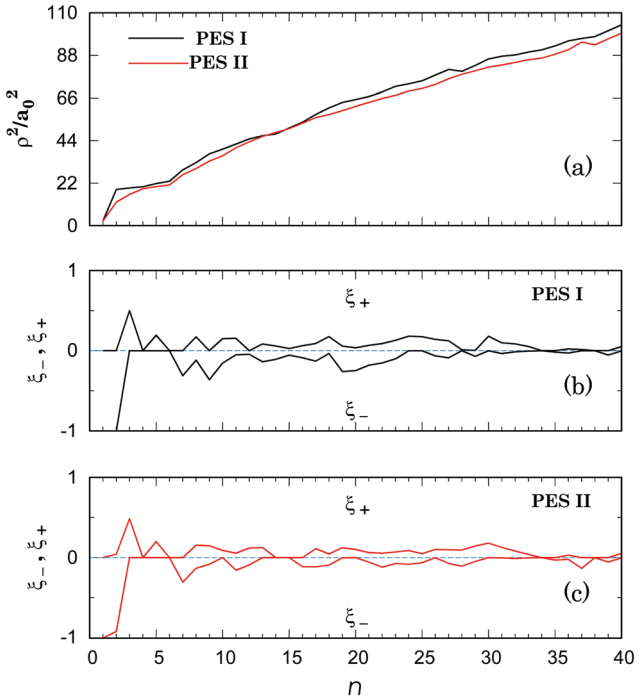

Fig. 7 Square of the hyperradius [panel (a)] and deformation indices [panel (b) for PES I and panel (c) for PES II] of the global minimum structures of the Li^+Ar_n (n = 1–40) clusters. In panel (a), the black curve is for PES I, while the red one refers to PES II. See the text.

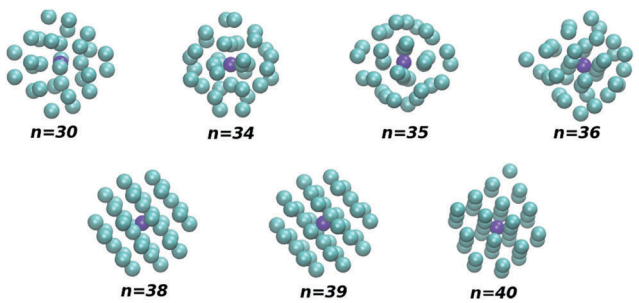

Fig. 8 Global minimum structures for large clusters that are similar in both PES I and PES II. The shapes of the clusters are oblate (n = 30 and 40), spherical (n = 34, 35 and 38) and prolate (n = 36 and 39).

The Royal Society of Chemistry apologises for these errors and any consequent inconvenience to authors and readers.

