Lawrence Berkeley National Laboratory

LBL Publications

Title

Correction: Enhanced 5f-8 bonding in [U(C 7 H 7) 2] – : C K-edge XAS, magnetism, and ab initio calculations

Permalink

https://escholarship.org/uc/item/4pj8d68x

Journal

Chemical Communications, 57(96)

ISSN

1359-7345

Authors

Qiao, Yusen Ganguly, Gaurab Booth, Corwin H et al.

Publication Date

2021-12-03

DOI

10.1039/d1cc90412d

Peer reviewed

Correction: Enhanced 5f-d bonding in [U(C7H7)2] : C K-edge XAS, magnetism, and ab initio calculations

Yusen Qiao,a Gaurab Ganguly,b Corwin H. Booth,a Jacob A. Branson,ac Alexander S. Ditter,a Daniel J. Lussier,ac Liane M. Moreau,a Dominic R. Russo,ac Dumitru-Claudiu Sergentu,b David K. Shuh,a Taoxiang Sun,a Jochen Autschbach*b and Stefan G. Minasian*a

Correction for 'Enhanced 5f-d bonding in [U(C7H7)2]: C K-edge XAS, magnetism, and ab initio calculations' by Yusen Qiao et al., Chem. Commun., 2021, 57, 9562–9565, DOI: 10.1039/D1CC03414F.

The authors regret that two references to the multi-configurational pair-density functional theory methods used in the wavefunction calculations did not appear in the main article. The references were included in the Methods section of the Electronic Supplementary Information as ref. 17a and b, but should also have appeared in the second paragraph on page 9564. The references are listed below as ref. 1 and 2. The Royal Society of Chemistry apologises for these errors and any consequent inconvenience to authors and readers. References 1 G. Li Manni, R. K. Carlson, S. Luo, D. Ma, J. Olsen, D. G. Truhlar and L. Gagliardi, J. Chem. Theory Comput., 2014, 10, 3669–3680. 2 R. K. Carlson, G. L. Manni, A. L. Sonnenberger, D. G. Truhlar and L. Gagliardi, J. Chem. Theory Comput., 2015, 11, 82–90.