Mechanochemical Synthesis of a Li-K Heterobimetallic Electride and its Versatile Reactivity

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Electride is a type of compound featuring free electrons as the anion [1]. As electron-rich materials, electrides could exhibit unusual physicochemical properties (such as electro-conductivity) underpinned by their electron density topologies [2]. So far, the reported electrides feature three types of electron density topologies: (1) zero-dimensional (0D) discrete cavities; (2) one-dimensional (1D) channels; (3) two-dimensional (2D) planes [3]. Recently, by employing mechanochemical ball milling, we synthesized the first electride with a three-dimensional (3D) helical electron density topology, namely $[LiHMDS][K^+][e^-]$ (**1**) (HMDS: $N(SiMe_3)_2$). Moreover, beyond the intriguing structural features, **1** exhibited versatile reactivity, enabling the first transition-metal free facile benzene (C_6H_6) coupling reaction, and the first solvent-free facile Birch-type reductions.

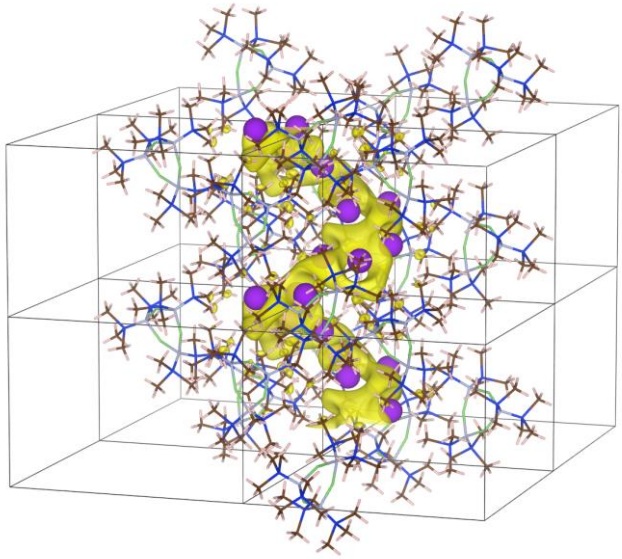

Fig. 1 3D Helical electron density topology in 1 from *A*b *I*nitio *R*andom *S*tructure *S*earching (AIRSS) calculations.

References:
[1] J. L. Dye, Electrides. *Scientific American* **257**, 66-75 (1987). Doi: 10.2307/24979479.
[2] J. L. Dye, Electrides: Early Examples of Quantum Confinement. *Acc. Chem. Res.* **42**, 1564-1572 (2009). Doi: 10.1021/ar9000857.
[3] C. Liu, S. A. Nikolaev, W. Ren, L. A. Burton, Electrides: a review. *J. Mater. Chem. C* **8**, 10551-10567 (2020). doi: 10.1039/d0tc01165g.

As a native of Hefei, China, Dr Erli Lu is a Newcastle University Academic Track (NUAcT) Fellow. Started at Newcastle in September 2019, the Lu group focuses on synthesising and characterising highly reactive group-1/2 metal complexes, and exploiting the group-1 metal solid-state chemistry (mechanochemical ball milling) in delivering low-carbon sustainable small molecule and material syntheses. Before joining Newcastle, Erli had worked in the Steve Liddle group at Nottingham (06.2012-10.2015) and Manchester (10.2015-06.2019) Universities, investigating actinide metal-ligand multiple bonds. Erli's PhD degree was awarded on 01.2012 by the Chinese Academy of Sciences, Shanghai Institute of Organic Chemistry (SIOC), for his work in rare-earth metal chemistry, specifically, rare-earth metal terminal imides, in the Yaofeng Chen group (09.2006-01.2012). Erli has published 35 papers (4 as the corresponding author at Newcastle) (h-index 21), 2 book chapters and 1 China patent. He was awarded the 5-year NUAcT fellowship (2019-24) to start an independent career, and the EU Marie Curie International Incoming Fellowship (2012-14), along with a few PhD/PDRA prizes/awards in China and the UK/EU.