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Supplemental Information: Electronic correlations and intrinsic magnetism of interstitial quasi-atomic states in Li_8Au electride

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1 HSE results and calculation details

Additional calculations with the HSE hybrid functional[1] were carried out to eliminate the self-interaction error and effectively takes into account the electron-electron interactions on all the states, including the *p*-Au. The calculations were performed on a uniform 4×4×4 *k*-mesh, for the Fock operator sampling a 2×2×2 *q*-mesh was used, the screening parameter was set to 0.1, and other settings were the same as for the main GGA calculations of Li_8Au. The resulting spin-polarized density of states is shown in Fig. 1. The different way of accounting for interactions leads to some differences between the HSE and DMFT related as expected primarily to the relative position of the *p*-band. But it is evident that the emergence of magnetic moments on electride states, as described by DMFT, is qualitatively reproduced by the hybrid functional, despite certain limitations and drawbacks of the latter.

Fig. 2 shows the isosurface of the spin-polarized charge density $\rho_\uparrow - \rho_\downarrow$ obtained using the HSE hybrid functional. It appears that the magnetization is provided by the electron density localized in the voids of the Li_8Au crystal lattice. It is noteworthy that no spin-polarized charge density is observed on the Au atoms. This is also consistent with the results of DFT+DMFT calculations, where the magnetic moments are observed to be localized on the intersite Wannier functions, localized in the centers of the Li-cubes. This suggests that despite the comparable band width with ISQ states, the correlation effects on *p*-Au states do not create any qualitative changes in the electronic structure of Li_8Au in the vicinity of the Fermi level.Thus, the minimal model we use, which considers only ISQ states as correlated impurity, does not miss any important effects related to the magnetic properties and behavior near the Fermi level.

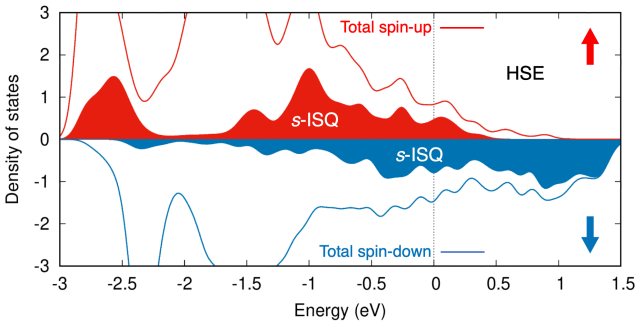

Fig. 1 Spin-resolved density of states of Li_8Au obtained by HSE calculation.

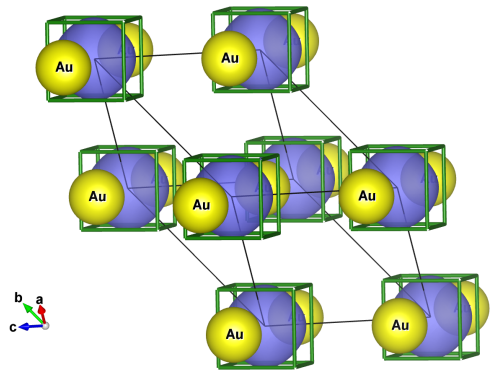

Fig. 2 Crystal structure of Li_8Au with isosurface of the spin-polarized charge density $\rho_\uparrow - \rho_\downarrow$ (in purple) obtained from the HSE calculation of LI_8Au. Li atoms are located in the vertices of the green-lined cubes.

Notes and references

1 J. Heyd, G. E. Scuseria and M. Ernzerhof, *The Journal of Chemical Physics*, 2003, **118**, 8207–8215.

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