DETAILED VIEW INTO THE Au_2^+ POTENTIAL ENERGY SURFACES

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Gold is a versatile material with unique properties that underpin its importance in medicine, catalysis, electronics and basic research. The theoretical description of even very small Au clusters remains challenging due to relativistic effects, d electrons participating in the bonding, spin-orbit coupling and charge-transfer effects. Using photodissociation spectroscopy, we have obtained the first optical spectrum of Au_2^+. The quality of the spectrum is high enough to allow a detailed analysis of the ground and excited state surfaces of this important model system.[1,2] The results presented show that standard TD-DFT methods completely fail to describe this seemingly simple, H_2^+ like system. Only with a relativistic multireference treatment including spin-orbit coupling were we able to obtain a qualitative agreement between experimental results and theory.

[1] M. Förstel et al., Angew. Chem. Int. Ed., 2020, 123, 21587-21592.
[2] M. Förstel et al., Rev. Sci. Instrum., 2017, 88, 123110.