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Innsbruck Physics Colloquium

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Dealing with Multiple Electronic States

As a single potential energy curve is often drawn in describing chemical processes, one might easily overlook the importance of other electronic states that might be reached from the ground electronic state or influence the system in a subtler way. The presence of multiple electronic states with a possible multiconfigurational character plays an important role in reactivity and spectroscopy. The effects are particularly prominent in transition metal systems, being thus of interest, *inter alia*, for catalysis, either in industrial applications or in biological systems (e.g., metalloenzymes).

In my talk, I will present the way one describes, numerically models and interprets systems in which multiple electronic states play a decisive role. These will include the properties of highly charged ions,[1] dissociative electron attachment,[2] and CO_2 activation on a Ta^+ ion.[3] Finally, I will show that the seemingly abstract *multiconfigurational character* of electronic states might be, under favorable circumstances, revealed spectroscopically.[4]

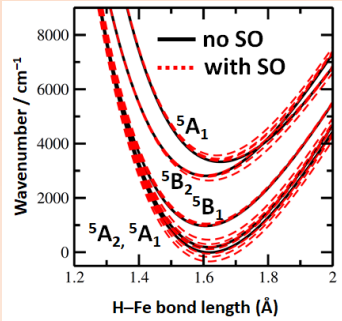

Figure 1 – The multitude of electronic states in FeH^+Ar_2.

[1] – L. Ganner, S. Bergmeister, L. Lorenz, M. Ončák, P. Scheier, E. Gruber, *Phys. Rev. Lett.*, 133, 023001 (2024). DOI: 10.1103/PhysRevLett.133.023001

[2] - F. Izadi, T. F. M. Luxford, B. Sedmidubská, E. Arthur-Baidoo, J. Kočišek, M. Ončák, S. Denifl, *Angew. Chem. Int. Ed.*, *in print*. DOI: 10.1002/anie.202407469

[3] - Y. Liu, M. Ončák, J. Meyer, S. G. Ard, N. S. Shuman, A. A. Viggiano, H. Guo, *J. Am. Chem. Soc.*, *146, 14182 (2024)*. DOI: 10.1021/jacs.4c03192

[4] – D. Jank, M. Ončák, S. Jin, C. van der Linde, M. K. Beyer, *J. Am. Chem. Soc., 24,* 16385-16388 (2024). DOI: 10.1021/jacs.4c05620

Tuesday, 01.10.2024, at 16:30 h, HS C (Technik)

Innsbruck Physics Colloquium,
Organisation: K. Erath-Dulitz, H.-C. Nägerl, T. Schrabback