Correlated Electron Materials – A Playground for Electronic Structure Theory

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Abstract. The field of electronic structure calculations for correlated materials has witnessed tremendous progress in recent years due to the development of combined electronic structure and many body theories. We will give an introduction to the concept of electronic correlations and the modeling thereof. Focussing on excited states properties, we will point out the need of going beyond band theory for correlated materials. We will summarize some of the main strategies of many-body theory and their combination with realistic electronic structure techniques. In particular, we will describe the ideas and formalism of dynamical mean field theory, and discuss its application in the electronic structure context. Finally, we will comment on current questions in the field and open challenges.

References

[1] Silke Biermann, *Dynamical mean field theory-based electronic structure calcualtions for correlated materials*, in: Topics in current chemistry, vol. 347, pp. 303-345, Springer (2014).

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