Controlling the Mott gap using substrates

Coulomb engineering of Mott insulators

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In Short

- How does the dielectric environment affect the Coulomb interaction and thereby the Mott gap?
- Use the environment to engineer desireable properties of monolayer Mott insulators
- Strong correlations and long-ranged interactions

Electrons are responsible for the charge transport in solids. The presence or absence of an energy gap at the Fermi level of the electrons determines if a material is insulating or metallic. Mott insulators are insulators where such a gap is caused by the Coulomb interaction between the (charged) electrons. In a vacuum, the strength of the Coulomb interaction depends only on the distance between the electrons in question. However, the electrons in real materials do not live in a vacuum and the Coulomb interaction is *screened* by other electrons in the material and its surroundings.

This kind of environmentally screening has the promise to be very interesting in Mott insulators, materials that should be conducting according to band theory, but where the electron-electron Coulomb interaction is sufficiently strong to localize the electrons and make the material insulating. Since the strength of the Coulomb interaction determines if such a system is insulating or metallic and is determined itself by the dielectric environment, this way to manipulate materials is called *Coulomb engineering*.

To study this effect in detail, we consider a thin layer of a Mott insulating material sandwiched in a dielectric environment, as illustrated in Figure 1. In this case, the Coulomb interaction $V(r)$ in the Mott insulator is screened by the environment: the field lines that pass through the environment will feel ε_E instead of ε_M. The screening changes the overall magnitude of the Coulomb interaction but it also changes how the interaction depends on the distance. Since the Coulomb interaction is responsible for many electronic properties and in particular for the Mott gap, in this situation the sandwich structure can be used to control these properties of the insulating monolayer: Coulomb engineering.

This scenario is hard to investigate theoretically and computationally. Due to the strong Coulomb interaction, the electrons in Mott insulators are *strongly correlated*. This means that the electrons cannot

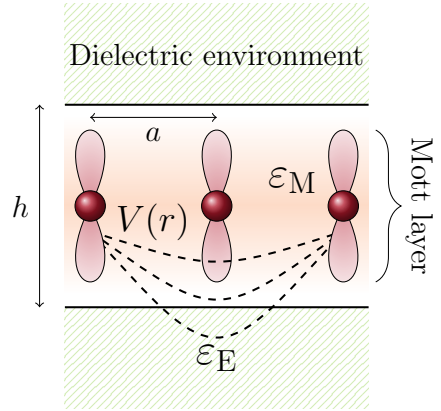

***Figure 1:** Impression of a monolayer Mott insulator on a substrate (not to scale). The Coulomb interaction $V(r)$ between electrons depends on the screening both inside the monolayer and by the substrate. This allows the substrate to be used as a tool to control the properties of the Mott insulator.*

be treated as independent particles and makes the electronic system difficult to treat computationally. A common approach is to use a simplified model, the Hubbard model, where only the interaction between electrons on the same site is taken into account. That simplified model is already extremely challenging to investigate numerically, but it is also cleary insufficient for this study since the spatial character of the environmental screening is essential.

This requires us to use the Dual Boson method [1], a modern many-body technique that can simultaneously deal with the strong short-ranged correlations that make the system insulating and with the long-ranged, environmentally screened Coulomb interactions. With this method, we have determined how the electronic spectrum of the Mott insulator depends on the environment.

Physicists study correlated electron systems by determining their *spectral function*. This spectrum shows if there are electronic states in the system with a given energy E and momentum k. Experimentally, the momentum-resolved spectral function can be investigated with angular resolved photoemission spectroscopy (ARPES), although ARPES only shows the part of the spectrum below the Fermi energy, and using scanneling tunneling spectroscopy (STS), which shows the average of the spectral function over all momenta. Theoretically, the spectral function is a natural output of the Dual Boson calculations.

Figure 2 shows how the calculated spectral function evolves from ε_E=1 (the monolayer is surrounded by vacuum) to an environmental dielectric constant

of ε_E=10 (bulk Si corresponds to ε_E=12). The colored curve on the right of each graph shows the density of states, the momentum average of the spectral function. The screening by the substrate leads to several substantial changes in the spectral function. Most dramatically, the system changes from an insulator to a metal: the gap at the Fermi level ($E = 0$) disappears and a quasiparticle band emerges there. These low-energy particles will be able to conduct, so that that system is not insulating anymore. The appearance of the quasiparticle peak is clearly visible both in the spectral function and the local density of states. On top of this dramatic change at Fermi level, the features further away are also clearly changing due to the environmental screening, with spectral intensity moving towards the Fermi level.

Our results demonstrate that the dielectric environment can be used to control Mott insulating layered materials, reducing the size of their Mott gap and even turning them into metals. Changes in the Hubbard bands and the size of the gap on the eV-scale are possible and a sufficiently strong dielectric environment can turn a Mott insulator conducting. Our work opens a perspective for the fabrication of heterostructures by the application of dielectric covering on parts of a Mott monolayer. In this way, conducting paths or quantum dots can be created in an otherwise insulating layer.

So far, we have proven the principle of Coulomb engineering: the environmental dielectric constant ε_E can produce an insulator-metal transition. Now, we wish to predict which Mott materials are most suited to Coulomb engineering, investigating the role of the internal screening of the material itself (ε_M) and the thickness of the monolayer material (h/a, the thickness compared to the interatomic distance). In addition to these material properties, the temperature is also expected to play an important role. We plan to investigate these aspects of Coulomb engineering in the near future.

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http://www.itp.uni-bremen.de/ag-wehling/

More Information

[1] E. G. C. P. van Loon, A. I. Lichtenstein, M. I. Katsnelson, O. Parcollet, and H. Hafermann, *Phys. Rev. B* **90**, 235135 (2014). doi: 10.1103/PhysRevB.90.235135

Project Partners

Prof. Dr. Sangiovanni (Universität Würzburg), Dr Springer and Dr. Tomczak (Technische Universität Wien)

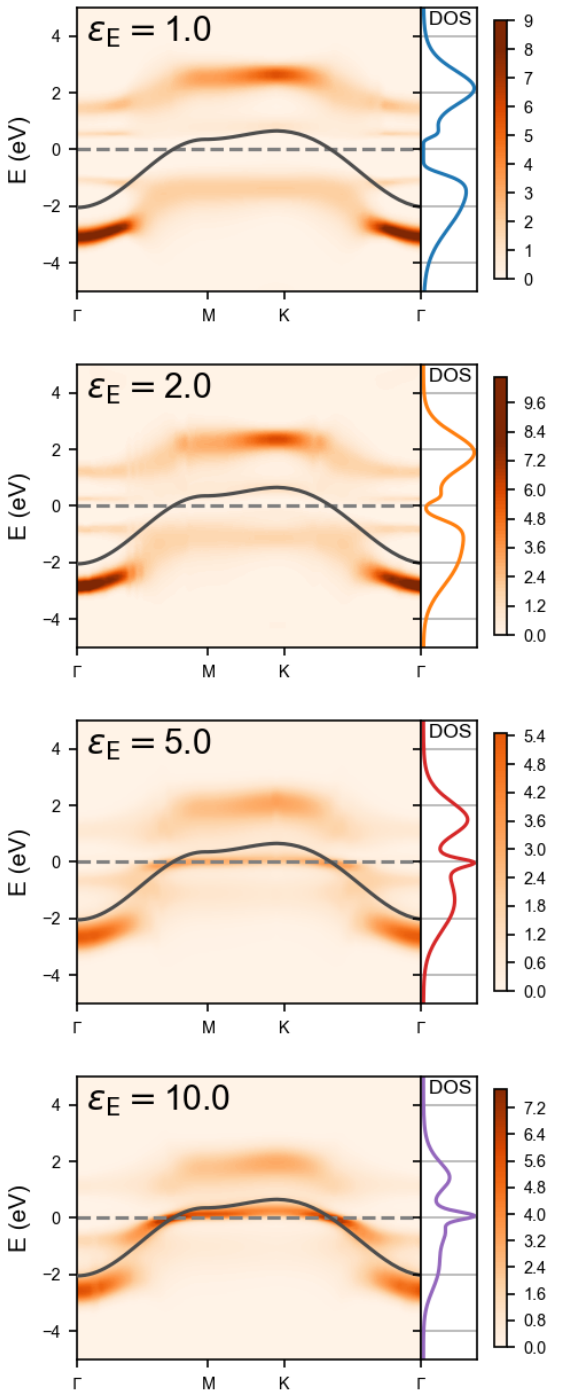

Figure 2: *Spectral function $A(k, E)$ of a monolayer surrounded by vacuum (ε_E=1) and by several dielectric environments (ε_E=2, ε_E=5 and ε_E=10). The Fermi level is at $E = 0$ (dashed line). The black curve is the non-interacting dispersion. On the right of both spectra, the corresponding local density of states (DOS) is shown. All calculations have been performed at an electronic temperature of 0.1 eV. The isolated monolayer is an insulator, with a gap in the spectrum around $E = 0$. When sandwiched by the dielectric, it turns into a metal with spectral weight at $E = 0$.*