

## Supplemental Material

### Extended regime of meta-stable metallic and insulating phases in a two-orbital electronic system

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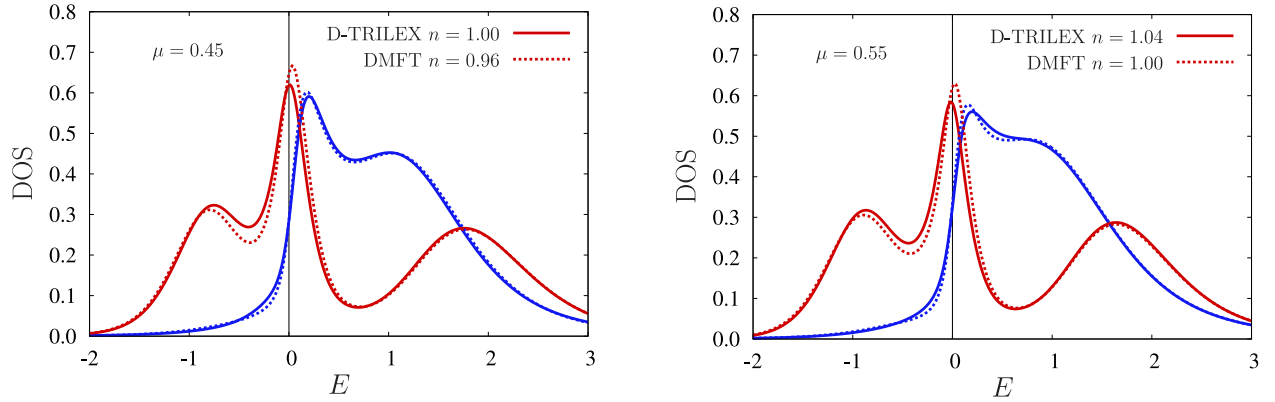


FIG. S1. DOS for the upper ( $l = 1$ , blue line) and lower ( $l = 2$ , red line) orbitals obtained for  $U = 2.4$  and  $J = U/6$  using D-TRILEX (solid lines) and DMFT (dashed lines) methods. Left panel corresponds to the chemical potential  $\mu = 0.45$  at which the D-TRILEX solution is quarter-filled ( $\langle n \rangle = 1.00$ ). Right panel corresponds to the chemical potential  $\mu = 0.55$  of the quarter-filled DMFT solution.

**Charge compressibility and meta-stability.** The meta-stability of the two solutions is signalled by the appearance of two different values of the chemical potential  $\mu$  and  $\mu^*$  leading to the same average density  $\langle n \rangle$ , as demonstrated in the left panel of Fig. 3 in the main text. As shown there, the presence of two meta-stable solutions manifest itself with the appearance of an hysteresis loop. The branch of the hysteresis chosen by the system depends on whether the corresponding reference system is metallic or Mott insulating. As a matter of fact, if we follow the  $\mu(U)$  curve that gives  $\langle n \rangle = 1$  in the weak coupling regime (red dots), we obtain the metallic solution until it continuously turns into an insulating phase at  $U_c$ . Above this threshold, any value of the chemical potential inside the Mott gap gives the same average density, and the two solutions corresponding to  $\mu$  and  $\mu^*$  can be considered equivalent from there on. On the other hand, if we start from the chemical potential  $\mu^*$  that corresponds to the insulating phase and decrease the interaction following the condition  $\langle n \rangle = 1$ , we obtain the insulating solution (red asterisks). The latter exists until the critical interaction  $U_c^*$  below which no solution for  $\mu^* \approx \mu^d$  is available at quarter-filling. This behavior means that the function  $\langle n \rangle(\mu)$  is not monotonic and exhibits a region of negative charge compressibility  $\kappa = \frac{1}{\langle n \rangle^2} \frac{d\langle n \rangle}{d\mu}$ . According to our calculations, the metallic and insulating D-TRILEX so-

lutions are both characterized by  $\kappa > 0$ , hence they are thermodynamically meta-stable. Since the density is the same for both phases, they have to be separated by a region of chemical potentials associated with a negative charge compressibility.

From the perspective of applications, this region of negative charge compressibility between the two meta-stable solutions could forbid the spontaneous switch between the two solutions. In this case, the application of a static electric field should be sufficient to drive the transition between the metallic and Mott insulating phases, as this perturbation would effectively change the chemical potential from  $\mu$  to  $\mu^*$  or *vice versa*. A similar switching between two meta-stable phases as a function of an electric field was investigated in Ref. [1], where a similar regime of parameters with coexisting metallic and Mott insulating meta-stable solutions was reported. One can speculate that the observed presence of two meta-stable phases could be exploited in the realization of Mott-based electronic switches or transistors. Indeed, the experimental realization of Mott field effect transistors (MottFET) was shown to be practically viable [2–4]. The simultaneous presence of metallic and Mott insulating states could be detected experimentally, for example by measuring dielectric properties of the system [5].

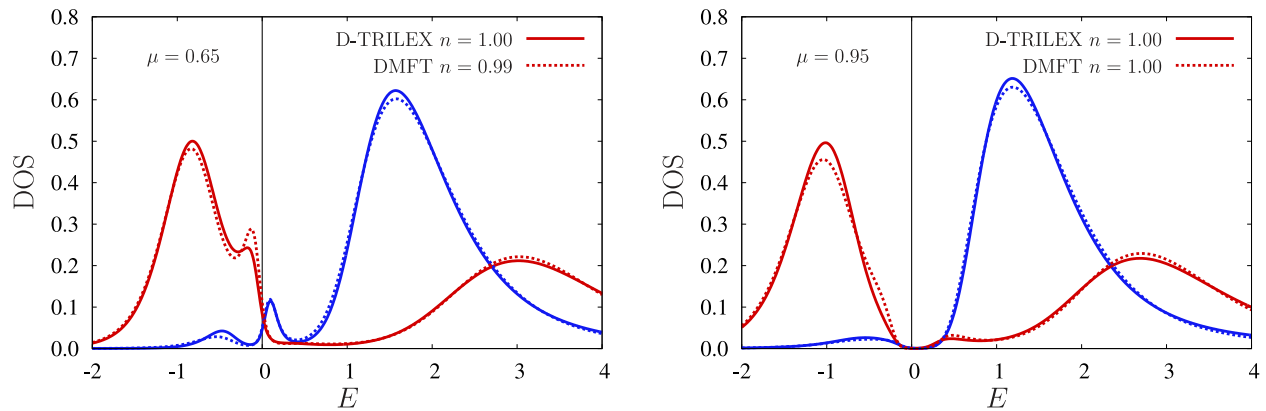


FIG. S2. DOS for the upper ( $l = 1$ , blue line) and lower ( $l = 2$ , red line) orbitals obtained for  $U = 4.2$  and  $J = U/6$  using D-TRILEX (solid lines) and DMFT (dashed lines) methods. Left panel corresponds to the chemical potential  $\mu = 0.65$  at which the D-TRILEX solution is metallic and quarter-filled ( $\langle n \rangle = 1.00$ ). Right panel corresponds to the chemical potential  $\mu = 0.95$  at which both, D-TRILEX and DMFT solutions are Mott insulating and quarter-filled.

**Calculations for a non-zero Hund’s coupling.** The quarter-filled ( $\langle n \rangle = 1$  electrons per lattice site) two-orbital model considered in the main text has a relatively big value of the crystal-field splitting. This leads to a large orbital polarization that appears already in the metallic regime before the system undergoes the Mott transition. The latter means that the single electron at each lattice site mostly populates the lower orbital ( $l = 2$ ), and the upper orbital ( $l = 1$ ) stays nearly unoccupied. In this case, it can be expected that including the Hund’s rule coupling  $J$  in the electronic interaction should not qualitatively change the physical effect observed in the absence of  $J$ . To confirm this point, we perform calculations for the local density of states (DOS) for two different interaction strength  $U = 2.4$  (Fig. S1) and  $U = 4.2$  (Fig. S2) for a non-zero value of the Hund’s coupling  $J = U/6$ .

Due to the effect of  $J$ , the system is still metallic at  $U = 2.4$  in contrast to the  $J = 0$  case, and we find a single value of the chemical potential  $\mu$  for which the D-TRILEX solution has an average density  $\langle n \rangle = 1$ . As in the case of  $J = 0$  discussed in the main text, the quarter filling in DMFT and D-TRILEX methods corresponds to different values of the chemical potential. At  $\mu = 0.45$  (left panel in Fig. S1), when the D-TRILEX solution is quarter-filled, the average density in DMFT is  $\langle n \rangle = 0.96$  electrons per lattice site. The chemical potential  $\mu = 0.55$  (right panel in Fig. S1) corresponds to the quarter-filled DMFT solution, while the average density in D-TRILEX is  $\langle n \rangle = 1.04$ . We find that both methods predict a rather similar DOS for each of the two values of the chemical potential. However, the average density of D-TRILEX is always larger than in DMFT. This observation is in agreement with the results reported in the main text for the case of  $J = 0$  and illustrates that in the metallic regime the role of the non-local fluctuations in the considered system consists in redistributing the spectral weight between the orbitals.

At  $U = 4.2$  the quarter-filled DMFT solution that corre-

sponds to  $\mu = 0.95$  lies in the Mott insulating regime (right panel in Fig. S2). For this value of the chemical potential the D-TRILEX solution is also quarter-filled and Mott insulating, because no spectral weight redistribution induced by the non-local fluctuations occurs in the insulating regime. Finally, at smaller value of the chemical potential  $\mu = 0.65$  (left panel in Fig. S2) the D-TRILEX reveals the second quarter-filled solution, which is metallic. The DOS predicted by DMFT for this value of the chemical potential is again similar to the one of D-TRILEX, but the DMFT solution does not reside at quarter filling and corresponds to  $\langle n \rangle = 0.99$ . Therefore, we find that when the DMFT solution becomes Mott insulating D-TRILEX reveals two different quarter-filled solutions even for the case of a non-zero value of the Hund’s coupling.

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