

DS 1: Organic Thin Films

Time: Monday 9:30–10:15

Location: REC/C213

DS 1.1 Mon 9:30 REC/C213

Thin film growth on weak surfaces: influence of substrate inhomogeneities — •ERIC KARAJIC¹, MARTIN OETTEL¹, EDWIN MOZO², and FABIO REIS² — ¹University of Tübingen, Institute of Applied Physics — ²Universidade Federal Fluminense, Instituto de Física

The initial island density in the growth of thin films on perfectly smooth surfaces is set by an interplay between flux, diffusion and the stability of small clusters [1]. However, real surfaces have inhomogeneities which may trap freely diffusion adsorbates and act as initial nucleation sites. Using kinetic Monte-Carlo (KMC) simulations, we investigate the influence of trapping strength and density of inhomogeneities on the initial growth behavior. We discuss the consequences for basic growth modes on weakly interacting surfaces [2]. For layer-by-layer growth, island densities may vary grossly between first and second layer, but for island growth the possible return to smooth growth at intermediate layer thicknesses is not affected. [1] T. Michely and J. Krug, Islands, Mounds, and Atoms, (Springer, 2003) [2] E. Empting et al., Phys. Rev. E 103, 023302 (2021)

DS 1.2 Mon 9:45 REC/C213

Organic self-assembled monolayers as barrier material in Josephson junctions — •MORITZ SINGER¹, HARSH GUPTA¹, RUI PEREIRA², BENEDIKT SCHOOF¹, and MARC TORNOW^{1,2} — ¹TU Munich, Garching, Germany — ²Fraunhofer EMFT, Munich, Germany

Superconducting qubits employ Josephson junctions (JJs) to provide the non-linearity needed to address a unique two-state system. The JJs consist of two superconducting electrodes which are separated by a nanometer-thin layer acting as tunnel barrier and is mostly fabricated from oxides. The thickness of the oxide is highly sensitive to process variations, and it hosts many two-level systems (TLS) which give rise to dielectric losses, thereby limiting the qubit coherence times. In this study, we report on JJs comprising an organic self-assembled monolayer (SAM) as the insulating barrier material. Our JJs consist of Ta electrodes on a Nb seed layer, separated by a SAM of octadecene (C₁₈H₃₆) molecules that are grown on the thin native TaO_x layer

of the bottom electrode. We fabricated JJs with three different electrode sizes in the μm - range and measured critical currents I_c between 3.7 μA and 30.6 μA at 100 mK, in good quantitative agreement with the expected values according to the Ambegaokar-Baratoff relation. We further analyzed the data using the Simmons tunneling model, adapted to account for the two-layer TaO_x/SAM barrier. We obtain barrier heights ranging from 0.43–0.57 eV for the SAM-JJs, which is significantly higher than for JJs fabricated with a Ta-oxide barrier only (barrier height 0.25 eV). This shows that the properties of JJs can be modified and tuned by introducing a SAM as barrier material.

DS 1.3 Mon 10:00 REC/C213

Prediction of room-temperature two-dimensional pi-electron half-metallic ferrimagnet — •JAN PHILLIPS¹, JOÃO C. G. HENRIQUES^{1,2}, ANTONIO T. COSTA^{1,3}, and JOAQUÍN FERNÁNDEZ-ROSSIER^{1,4} — ¹International Iberian Nanotechnology Laboratory (INL), Av. Mestre José Veiga, 4715-330 Braga, Portugal — ²Universidade de Santiago de Compostela, 15782 Santiago de Compostela, Spain — ³Universidade do Minho, R. da Universidade, 4710-057 Braga, Portugal — ⁴On permanent leave from Departamento de Física Aplicada, Universidad de Alicante, 03690 San Vicente del Raspeig, Spain

We propose a strategy to obtain conducting organic materials with fully spin-polarized Fermi surface, lying at a singular flat band, with antiferromagnetically coupled magnetic moments that reside in π -orbitals of nanographenes. We consider a honeycomb crystal whose unit cell combines two molecules with $S=1/2$: an Aza-3-Triangulene, a molecule with orbital degeneracy, and a a 2-Triangulene. The analyzed system is half-metallic with a ferrimagnetic order, presenting a zero net total magnetic moment per unit cell. We combine density functional theory calculations with a Hubbard model Hamiltonian to compute the magnetic interactions, the bands, and the collective spin excitations. We obtain very large intermolecular exchange couplings, in the range of 50 meV, which ensures room temperature stability. This crystal being a half-metal with fully compensated magnetic moments combines two characteristics that would make it ideal for spintronics applications.