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# AB-Intitio Study of OLED Electrodes for the Fundamental Application and Properties by Using Density Functional Theory Approach

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Organic Light Emitting Devices (OLEDs) have long used indium tin oxide (ITO) as a highly-transparent, conducting anode for the case of polymer light-emitting devices, a metal cathode with a low work function has also been necessary for the attainment of facile electron injection and efficient device operation. Due to the fact that the power efficiency of OLEDs can exceed that of incandescent lamps, discharge lamps, lighting purposes is very promising with organic layers prepared in vacuum from low molecular weight organic semiconducting materials. In contrast to that, the established liquid crystal displays only changes the polarization state of the illuminating light, an effect which is strongly viewing angle dependent and the lowering of the operating voltages of OLEDs. The field of organic semiconductors comprises also an additional field, namely polymeric semiconductors. It will explode with the availability of high resolution large and flat organic displays, capable of displaying information at video rates, operating at low voltages and consuming very little energy, which makes them suitable for battery powered purpose. In order to develop a novel and efficient OLEDs, in our work emphasis will be given to internal properties especially electronic properties of electrodes (Graphene, Alq3 Super yellow, PEDOT:PSS etc.) and active medium. For which, a density functional based SIESTA (Spanish Initiative for Electronic Simulations with Thousands of Atoms) and TRANSIESTA for the measurement of different properties.

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