Time dependent density functional study of enhanced field emission from carbon nanotubes

JOSEPH DRISCOLL, KALMAN VARGA, Vanderbilt University, Nashville — We have calculated the field emission current of carbon nanotubes in real-time and real-space using the Lagrange- function basis [1] combined with efficient time-propagating schemes. Experimental studies reported orders of magnitude increase of field emission current from Cesium deposited carbon nanotubes [2]. We have studied the increase of field emission current due to the deposition of different atoms (Cesium, Gold, Tungsten, etc.) on capped carbon nanotube tips. The theoretical results are in good agreement with the experimental findings. This work was supported by NSF grant ECS 0622146.