Abstract Submitted for the MAR05 Meeting of The American Physical Society

First-principles simulation of the field emission from noble metal nanowires CHOONG-KI LEE, JISOON IHM, School of Physics, Seoul National University, Seoul, Republic of Korea — We carry out a theoretical study on the field emission from the nanowire which is composed of noble metal elements such as silver or gold. Our calculations are based on the first-principles density functional theory within a localized basis scheme using the SIESTA package. Electronic states and the potential of the system under finite applied voltages are determined self-consistently. Through explicit time evolution of the wavefunction, we obtain the emission current and the shape of the charge density distribution of the emitted electrons from noble metal nanowire tip.

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Date submitted: 29 Nov 2004

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