Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

Why Is The Size Dependence Of the Scanning Tunneling Microscopy Workfunction Order Of Magnitude Larger Than That Of Photoemission ? WEI-XUE LI, XIN LIU, Dalian Insitute Of Chemical Physics, CAS, Dalian, China, S.B. ZHANG, National Renewable Energy Laboratory, Golden, CO, U.S.A. — Quantum size effect (QSE) has been studied extensively, as a primary driving force for nano technology. Recent scanning tunneling microscopy workfunction of ultrathin Pb(111) film found however order of magnitude larger of QSE than that of photoemission. By first-principles calculations, we show that the QSE is not merely a size effect but symmetry driven: being maximal at the $\overline{\Gamma}$ point (i.e., the center of the surface Brillouin zone) derived from interlayer coupling of p_z orbital, but could be vanishingly small at other symmetry points from in-plane $p_{x,y}$ orbital. The $\overline{\Gamma}$ valley states have the slowest decay. Thus they are the ones being picked up by near-field techniques such as the scanning tunneling spectroscopy. While whole surface Brillouin zone contributes equally to photoemission, and only marginal QSE effect occurs. For this reason, symmetry could be essential for all near-field physics and chemistry.

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Date submitted: 28 Nov 2007 Electronic form version 1.4