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First principles calculations of field emission from a defected metal surface

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Small surface defects are thought to affect field emission through the field enhancement and modification of the work function. We combined density functional theory and quantum transport calculations to study the influence of atomic–scale defects on the work function and field emission characteristics of copper surfaces. A newly developed general methodology for the calculation of the field emitted current density from nano-featured surfaces is used to study specific defects on a Cu(111) surface.
Our results show that the inclusion of a defect can significantly locally enhance the field emitted current density. However, this increase is attributed solely to the decrease of the work function due to the defect, with the effective field enhancement being minute. Finally, the Fowler–Nordheim equation is found to be valid when the modified value for the work function is used, with only an approximately constant factor separating the computed currents from those predicted by the Fowler–Nordheim equation

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