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**Explaining the electroluminescence of single molecules**<sup>1</sup> JOHN BUKER, GEORGE KIRCZENOW, Simon Fraser University — Experimental studies of electroluminescence from molecules on complex substrates have yielded intriguing relationships between the current-voltage characteristics and optical emission from such systems.<sup>2</sup> In this talk we propose a theoretical model that is able to account for many observed properties of these systems. We obtain distinct photon emission spectra and corresponding I-V curves for different couplings of the electrodes to the molecule, that are consistent with experimental data. We find emission to be highly dependent on the details of the tip/molecule and molecule/substrate coupling, and make further photon emission predictions for systems not yet achieved experimentally.

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<sup>2</sup>X. H. Qiu, G. V. Nazin, W. Ho, Science **299**, 542 (2003), S. W. Wu, N. Ogawa, W. Ho, Science **312**, 1362 (2006).

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