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Ligand-receptor binding kinetics in surface-plasmon resonance devices: A Monte Carlo simulation study[1] MATTHEW T. RAUM, Department of Physics, Virginia Tech, Blacksburg, VA 24061-0435, MANOJ GOPALAKRISHNAN, Harish-Chandra Research Institute, Allahabad 211019, India, KIM FORSTEN-WILLIAMS, Department of Chemical Engineering, Virginia Tech, Blacksburg, VA 24061, UWE C. TAUBER, Department of Physics, Virginia Tech, Blacksburg, VA 24061-0435 — We use lattice Monte-Carlo simulations to probe the kinetics of ligand-receptor association and dissociation. Simulations were run under conditions approximating the geometric configuration of surface plasmon resonance devices. These conditions include viscous flow of ligands over a surface of receptors which is achieved by using a spatially varying biased random walk. Our simulations allow for the occurrence of multiple rebinding events which result in strong deviations from the standard mean-field rate equation approximation. Our simulations also allow us to test improved theoretical predictions for the binding dynamics and to determine their range of applicability.

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Uwe C. Tauber
Department of Physics, Virginia Tech, Blacksburg, VA 24061-0435

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