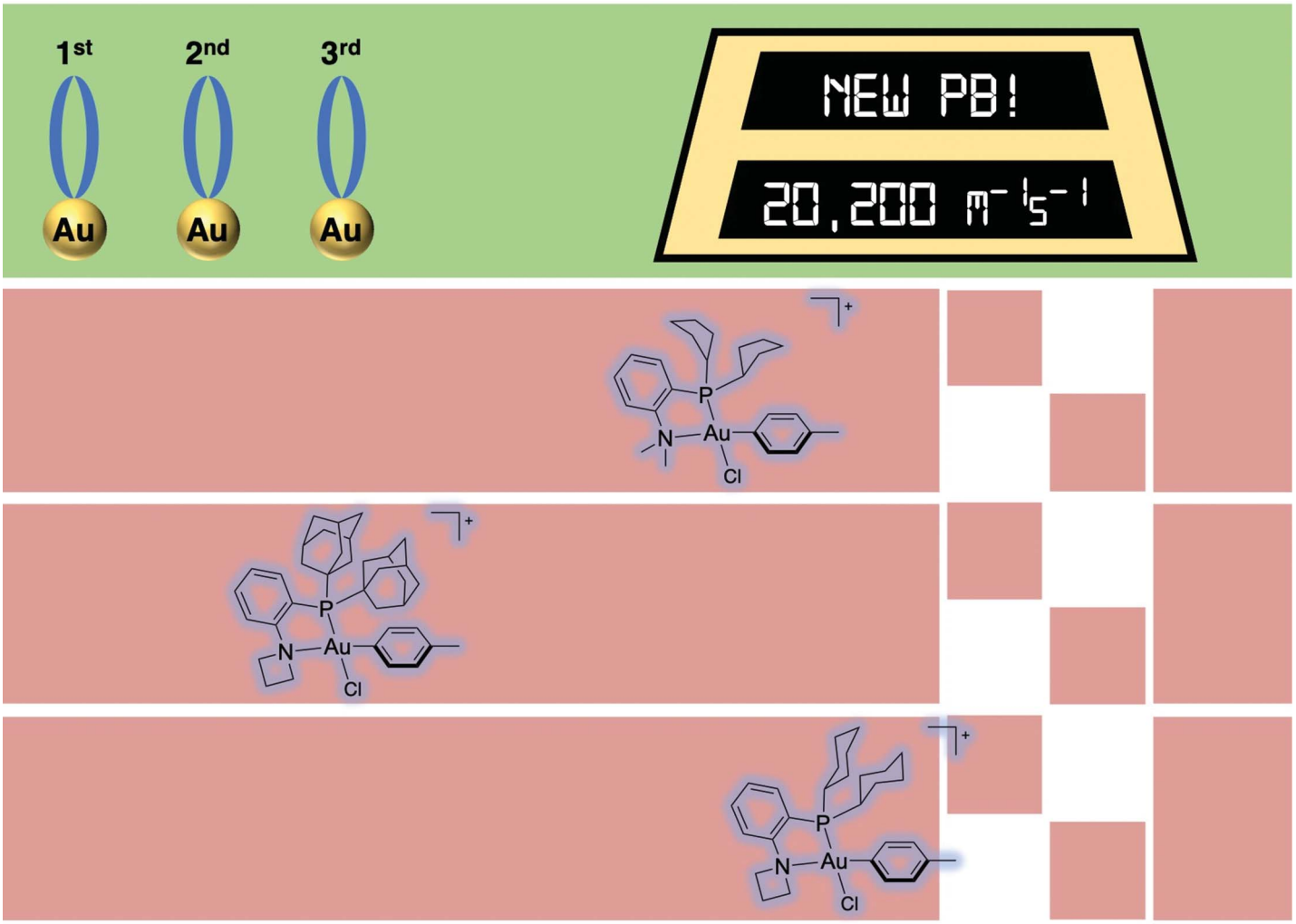

Showcasing research from Professors Heather Maynard's, Kendall Houk's, and Alexander Spokoyny's Laboratories, Department of Chemistry and Biochemistry, UCLA, Los Angeles, CA, USA.

In silico screening of *P,N*-ligands facilitates optimization of Au(III)-mediated *S*-arylation

Our study demonstrates how modifying the *P,N*-ligand on Au(III) oxidative addition complexes affects the kinetics of both elementary steps of the Au(III)-mediated *S*-arylation reaction. Computational screening identified three synthetically accessible *P,N*-ligands that were experimentally determined to have bimolecular coordination rate constants from 11,600–20,200 $M^{-1}s^{-1}$.

As featured in:

See Alexander M. Spokoyny, K. N. Houk, Heather D. Maynard *et al.*, *Chem. Sci.*, 2025, **16**, 3878.

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