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# Excimontec v1.0: An Open-Source Software Tool for Kinetic Monte Carlo Simulations of Organic Electronic Devices

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**Software**

- Review
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## Summary

For over three decades, kinetic Monte Carlo (KMC) simulations have been a powerful computational tool to help understand and optimize organic semiconductor devices, especially photovoltaics, light-emitting diodes, transistors, and thermoelectrics.(Baranovskii, 2014; Groves, 2017; Heiber et al., 2019; Zuo, Abdalla, & Kemerink, 2019) KMC simulations allow the construction of a detailed mechanistic model for how excitons and polarons are created, migrate through, and are then eventually removed from the semiconductor layer of a device and can capture the complex interactions between performance and spatial structure that is often not possible using continuum drift-diffusion models. Despite the clear utility of the method, no widespread or standardized software tools have taken hold in the community. Instead, many research groups around the world have maintained private codebases of varying complexity, efficiency, and reliability. As a result, there have been large barriers to entry for new researchers and a lot of repeated effort throughout the community that would have been much better off applied to pushing the capabilities of the technique and further refining the physical models.

`Excimontec` is designed to be a well-tested, optimized, reliable, and accessible open-source tool for performing KMC simulations of organic electronic devices. v1.0 has a particular focus on organic photovoltaic device modeling and can utilize complex bulk heterojunction morphologies generated using the `Ising_OPV` tool.(Heiber, 2019a) The software is being developed in modern C++ and is optimized for efficient execution on high performance computing clusters using MPI. This software package uses object-oriented design and extends the `KMC_Lattice` framework.(Heiber, 2019b) The code includes rigorous unit testing with `googletest`, integration testing with `TravisCI`, and API documentation generated using `Doxygen`. The source code for `Excimontec v1.0` is archived with Zenodo.(Heiber, 2020)

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