# Simulation tools within VIPERLAB

| Name | Category | Back end software needed? | input files | output files | Partner | Contact | open source ? | cluster or desktop PC? | typical single simulation duration [min.] | specialities |
|---|---|---|---|---|---|---|---|---|---|---|
| CROWM | optical | Matlab | text files containing thicknesses, n&k and optionally textures and variable excitation spectra | text files; absorption spectra of each layer /EQE, photo current (losses) | EPFL | christian.wolff@epfl.ch | no | both | 1 | ray-tracing for texturing |
| SCAPS 1D | electrical | no | text files; mobilities, trap densities, thicknesses,.. | text files containing JV, CV, Cf,.. | EPFL | christian.wolff@epfl.ch | yes | PC | 1 | |
| SIMsalabim | electrical | free pascal | text files; mobilities, trap densities, thickn., ilumination intensity.. | text files; JV, e.g. scan-rate/-direction dependent | EPFL | christian.wolff@epfl.ch | yes | both | 1 | includes mobile ions (2 species) |
| SILVACO | opto-electrical | no | text files: illumination spectrum, refractive indexes.... | text files + able to visualize them with the program | CENER | ezugasti@cener.com | no | desktop PC | 1-30 min | |
| CROWM | optical | Matlab | text files: layers materials & thicknesses, n&k profiles, surface textures, … | text files: RAT spectra of each layer /EQE, photo current (losses) | CEA | david.pelletier@cea.fr | no | both | 1 | Ray-tracing for texturing |
| SILVACO | opto-electrical | no | text files: layers structures & properties, mobilities, doping level, n&k profiles, … | text files: IV curves, band diagram | CEA | david.pelletier@cea.fr | no | both | 1-30 min | |
| TIBERCAD | opto-electrical | no | text files: mesh file, material parameter files, simulation input file, optionally: generation profiles, doping profiles | in 1D text files, in 2/3D VTK: IV curves, spatial data (band edges, densities, ...), generation profile | UNITOV | auf.der.maur@ing.uniroma2.it | no (might change soon) | both | 1-10 min (1D), 10 min - hours (2/3D) | multi-particle drift-diffusion, possible linking to thermal and QM modules, developed at UNITOV |
| COMSOL | optical (FEM and ray tracing) | no | GUI based | fields, generation rate | UNITOV | auf.der.maur@ing.uniroma2.it | no | both | >1 | available modules: full wave and ray tracing, can be combined |
| CST Microwave Studio | optical (FDTD) | no | GUI based | spatial data: fields, absorbed power | UNITOV | auf.der.maur@ing.uniroma2.it | no | both | 10 min - hours | |
| Sentaurus TCAD | opto-electrical | no | GUI based, parameter text files, physical models,... | various (e.g. band diagram, generation, recombination, JV/EQE, tunnel currents, ion/carrier distributions, currents, many more) | Fraunhofer ISE | christoph.messmer@ise.fraunhofer.de | no | both | 1min to 1day | detailed modelling, drift-diffusion including ions, tunnel models (e.g. trap assisted tunneling), thin film optics + ray tracing |

| Quokka3 | electrical | no | Silicon bulk properties (doping, lifetime)<br>Skin: sheet resistance, recombination current (also with lateral variation)<br>metallization: geometry, contact resistance, finger resistance)<br>optics: illumination spectrum, various options for optical models<br>Top cell: IV curve or 2-diode model parameters, EQE | IV curve+parameters, EQE, current and power loss analysis, luminescence (Si), 3D distribution of voltage/current etc. | Fraunhofer ISE | andreas.fell@ise.fraunhofer.de | no | cluster | 1-30 min | simulation of lateral cell effects, simulation of perovskite top cell as 1D skin |