Sensitivity Analysis for an Electron Transport System

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Research Area

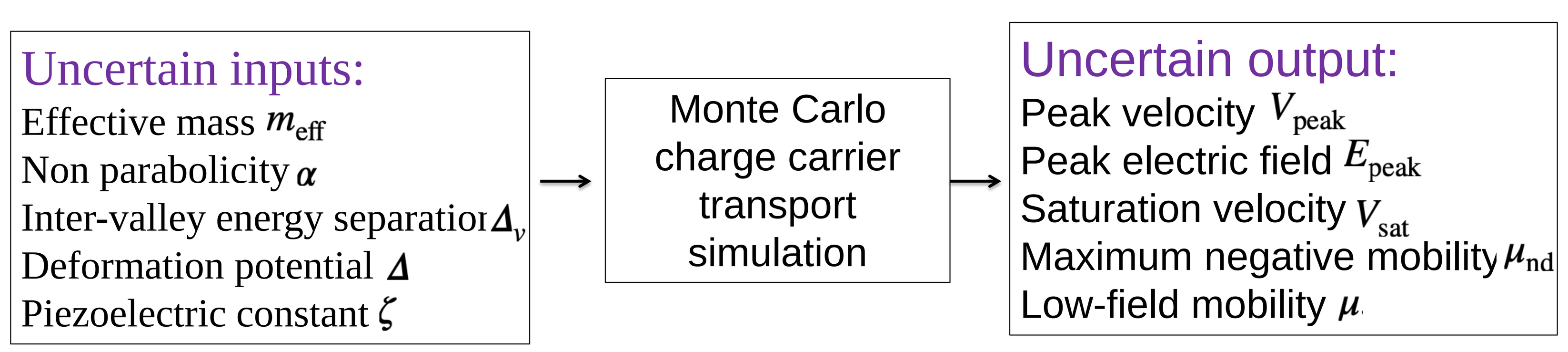
In the study of the transport of charge carriers (electrons and holes) within semiconductors, ensemble Monte Carlo simulations have been widely used for predicting the transport properties of emerging materials and thereby providing a framework within which expected device performance can be optimized. Associated with a given Monte Carlo charge carrier transport simulation, a large number of material and band structural parameters must be specified, these shaping the character of the resultant charge carrier transport results. However, some of these parameters are not very well known, or have yet to be experimentally measured or estimated through theoretical argument.

Goals

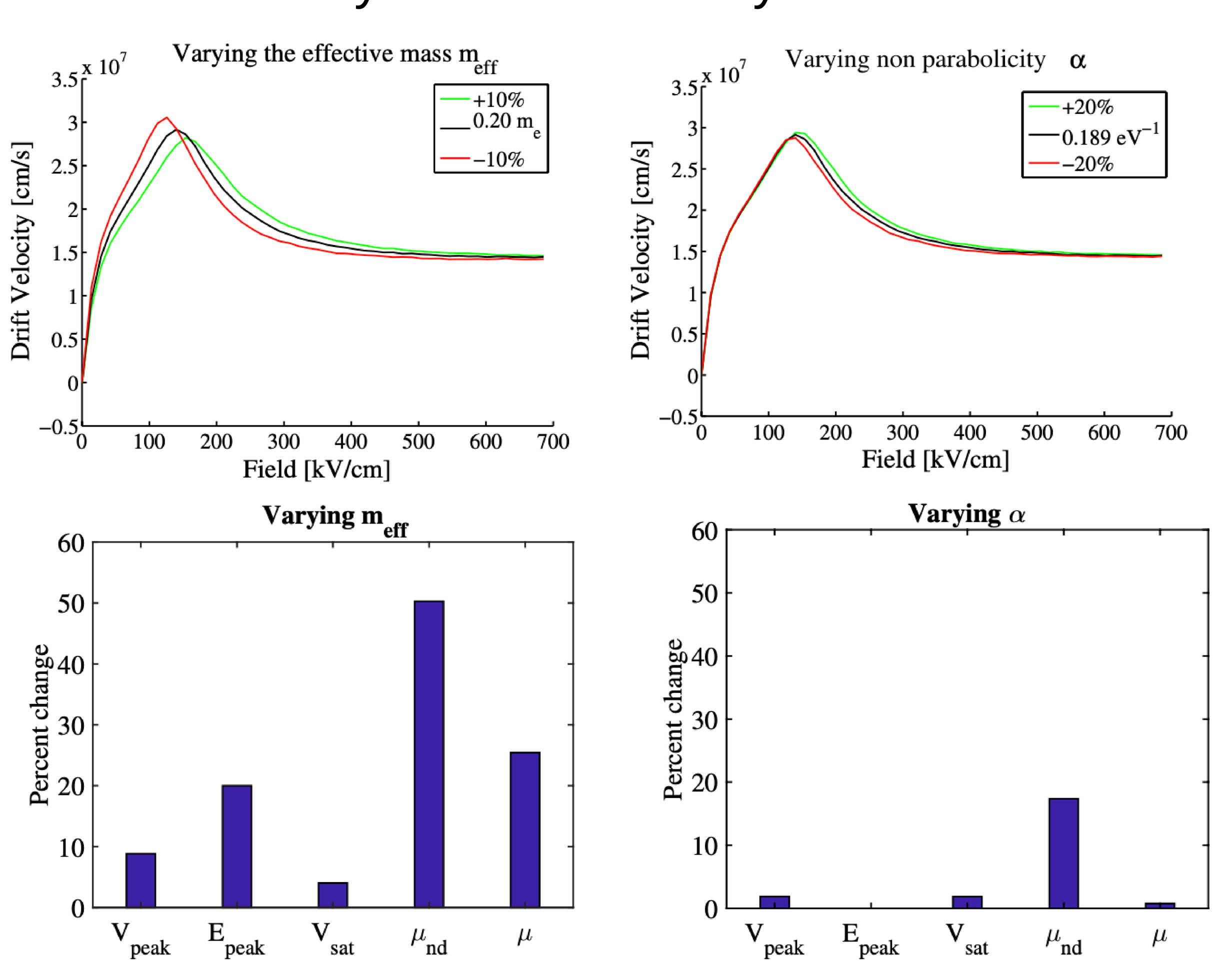
- Quantify the uncertainty in material and structural parameters using uncertainty quantification techniques.
- Identify the key parameters that strongly affect the transport properties.

Current State and Challenges

➢ Monte Carlo simulation of electron transport



➢ Intuitive analyses for sensitivity



Velocity field curves by varying effective mass by 10% (left) and non parabolicity by 20% (right)

Percent of change in transport properties by varying effective mass by 10% (left) and non parabolicity by 20% (right)

➢ Challenge

- Intuitive analyses use only partial information of uncertain inputs, therefore may not provide accurate sensitivity results.

Strategy

➢ Local sensitivity analysis

Let u denote individual transport property, ξ_i be the i[th] input.

the local sensitivity analysis of u with respect to ξ_i is

$$\mathrm{LSA}_i = \frac{\xi_i}{u} * \frac{\partial u}{\partial \xi_i} \approx \frac{\xi_i}{u} * \frac{\Delta u}{\Delta \xi_i}$$

➢ Global sensitivity analysis (identify "important" uncertain parameters)

ANOVA (analysis of variance) decomposition

$$u(\xi) = u_0 + \sum_i u_i(\xi_i) + \sum_{i<j} u_{ij}(\xi_i, \xi_j) + \ldots + u_{1,\ldots,n}(\xi_1, \ldots, \xi_n),$$

where

$$\int u(\xi) d\xi = u_0, \quad \int u(\xi) \Pi_{k \neq i} d\xi_k = u_0 + u_i(\xi_i),$$

$$\int u(\xi) \Pi_{k \neq i,j} d\xi_k = u_0 + u_i(\xi_i) + u_j(\xi_j) + u_{ij}(\xi_i, \xi_j),$$

$$\vdots$$

The variance of $u_{i_1, i_2, \ldots, i_r}$ is

$$D_{i_1, i_2, \ldots, i_r} = \int u^2_{i_1, i_2, \ldots, i_r} d\xi_{i_1, i_2, \ldots, i_r},$$

The total variance is

$$D = \int u^2(\xi) d\xi - u_0^2 = \sum_{r=1}^{n} \sum_{i_1 < \ldots < i_r}^{n} D_{i_1, i_2, \ldots, i_r}$$

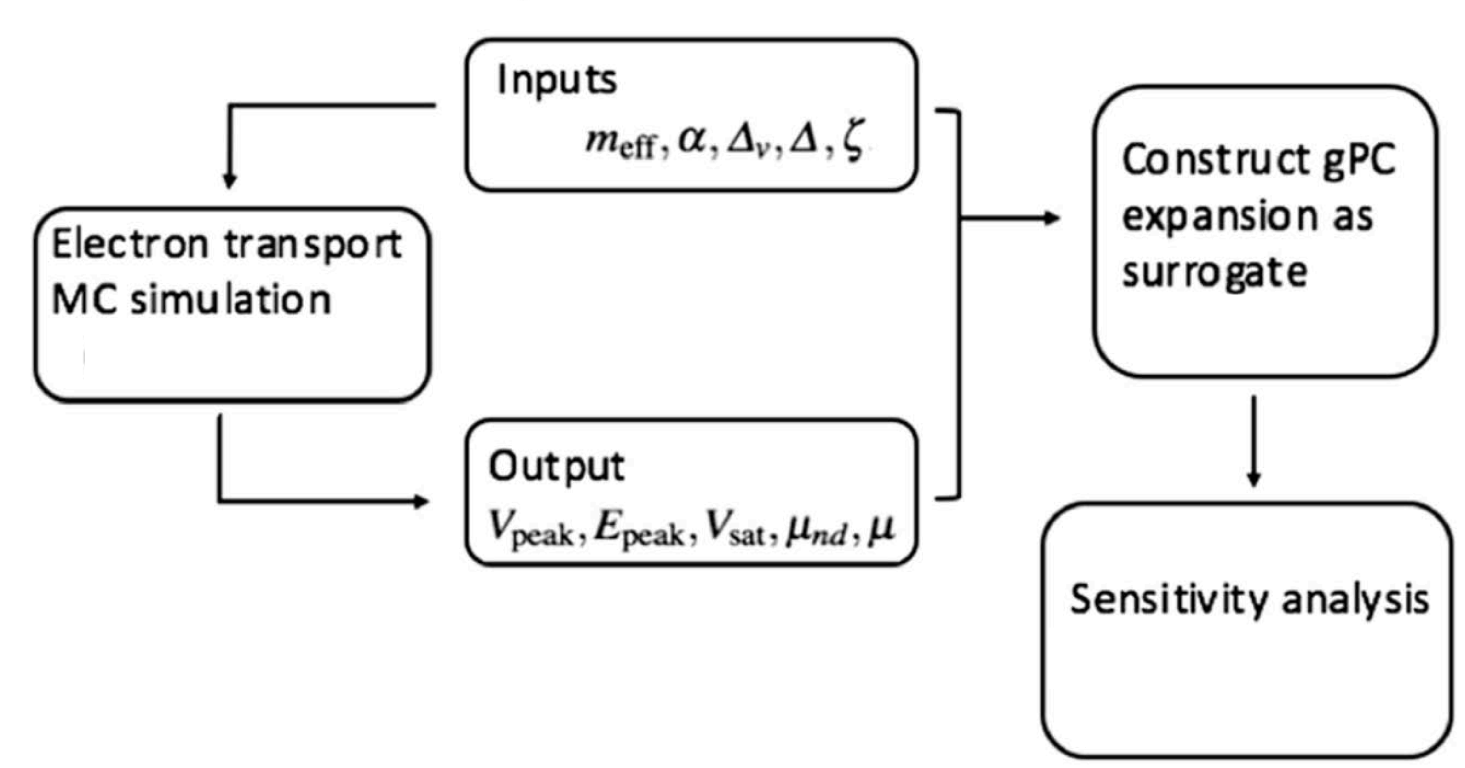
The Sobol index (global sensitivity index)

$$S_{i_1, i_2, \ldots, i_r} = D_{i_1, i_2, \ldots, i_r} / D$$

➢ Generalized polynomial chaos expansion

$$u(\xi) \approx u_p(\xi) = \sum_{i=0}^{N-1} u_i L_i(\xi),$$

Flow chart of the algorithm for Sobol indices evaluation



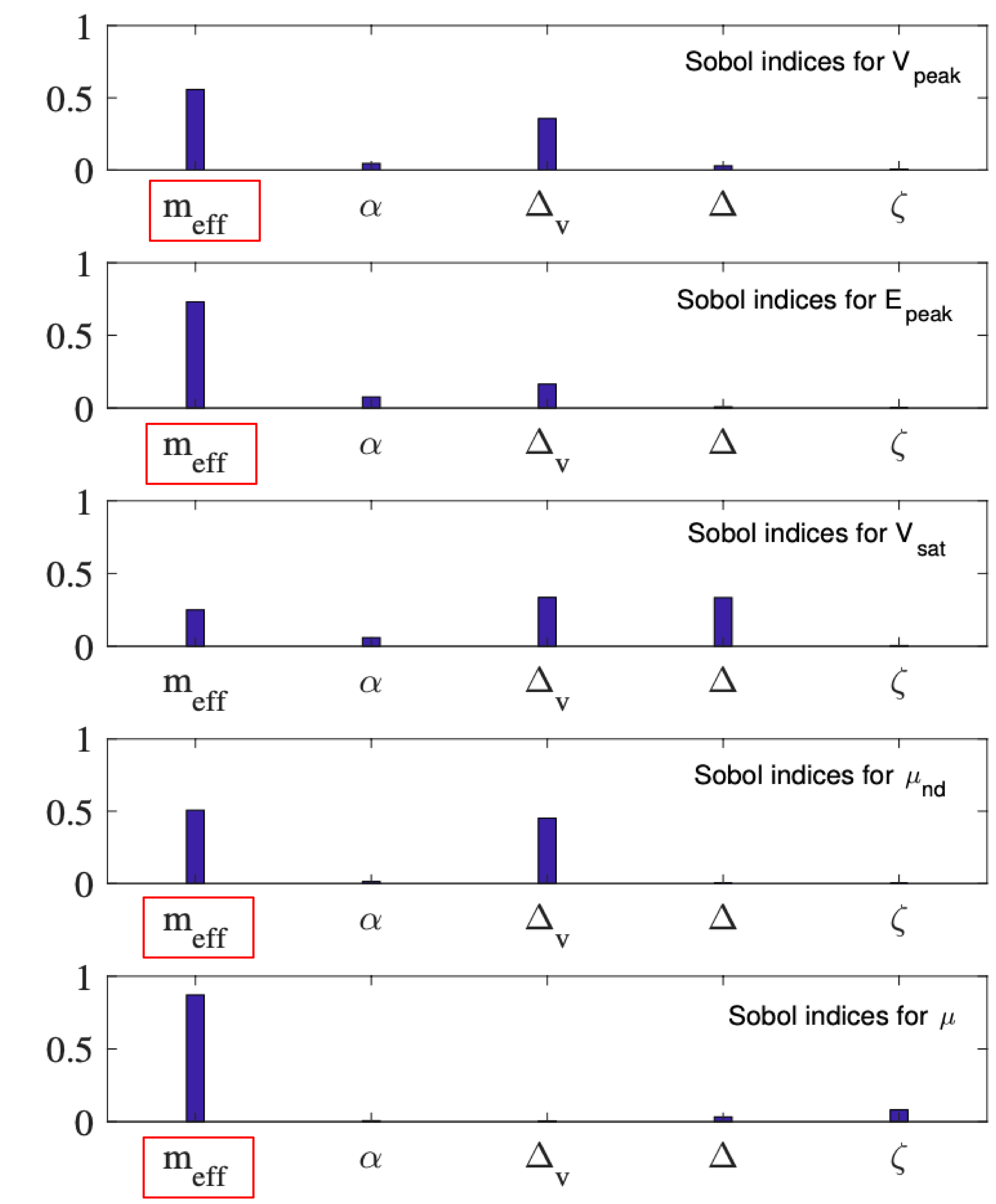
Significant Accomplishments

➢ Local sensitivity analysis results

Inputs \ QoIs	V_{peak}	E_{peak}	V_{sat}	μ_{nd}	μ
m_{eff}	0.442	1	0.202	2.51	1.27
α	0.047	0	0.047	0.434	0.0189
Δ_v	0.096	0.167	0.074	0.709	0.0067
Δ	0.049	0	0.113	0.115	0.2842
ζ	0.034	0	0.016	0.086	0.1974

Table 1 Local sensitivity analysis of each transport property (or QoI) with respect to each uncertain input parameters

➢ Global sensitivity analysis results



Effective mass is the key factor

Publication

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