The LisbOn KInetics computational tool

LoKI

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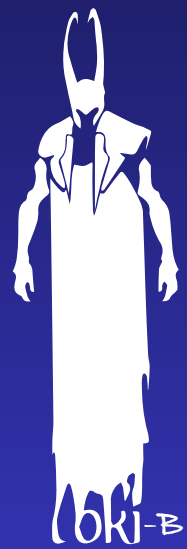
Introduction
KIT-PLASMEBA
LoKI
The code
How to use the code?
The benchmarks
Atomic gas: He
Molecular gas: N_2



Outline

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- LoKI

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- How to use the code?

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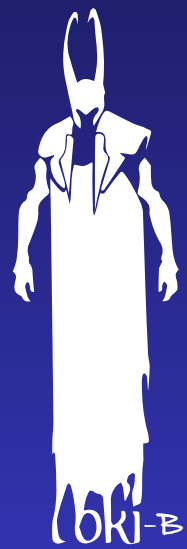

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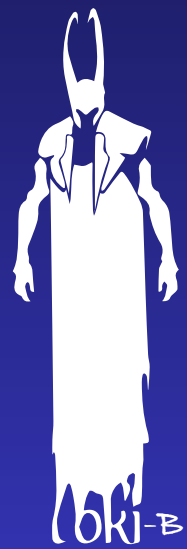


The KIT-PLASMEBA project

Framework of development of LoKI

- The LoKI tool is being developed in the framework of the KIT-PLASMEBA (KInetic Testbed for PLASMa Environmental and Biological Applications) project.

KIT-PLASMEBA

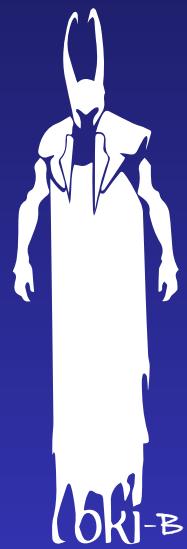
- aims constructing an open-source kinetic code for N_2-O_2 mixtures (in presence also of rare gases)
- providing the combined chemical and transport description of plasma charged / neutral species, both in volume and surface phases
- user-defined mixture compositions, pressure, radial dimension and excitation conditions.

FCT Fundação para a Ciência e a Tecnologia

MINISTÉRIO DA CIÊNCIA, TECNOLOGIA E ENSINO SUPERIOR

Ref.: PTDC/FISPLA/1243/2014

http://plasmakit.tecnico.ulisboa.pt



The KIT-PLASMEBA team

People behind the development of LoKI

The Modelling and Simulation (M&S) team within the "N-Plasmas Reactive: Modelling and Engineering" (N-PRiME) of Instituto de Plasmas e Fusão Nuclear (IPFN)

Permanent Staff

L. L. Alves, **PI**
- Boltzmann
- Ion transport

V. Guerra
- Kinetic schemes

C. D. Pintassilgo
- Thermal model

L. Marques
- Neutral transport

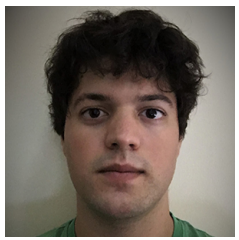
N. R. Pinhão
- Web access

M. Lino da Silva
- Web access
- Documentation

Post-Doc

A. Tejero-Del-Caz
- Main developer of LoKI (LoKI-B+LoKI-C)

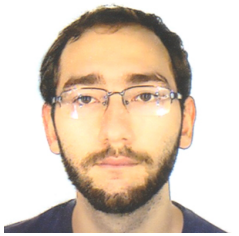
Students



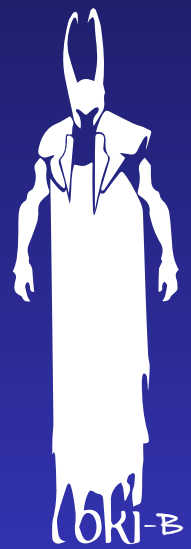
D. Gonçalves
- Ionization and e-e collisions (LoKI-B)

A. Silva
- O_2/O kinetics (LoKI-C)

S. Jacob
- N_2/N kinetics (LoKI-C)



D. Nina
- Draft version of LoKI-C



The LoKI simulation tool

LoKI

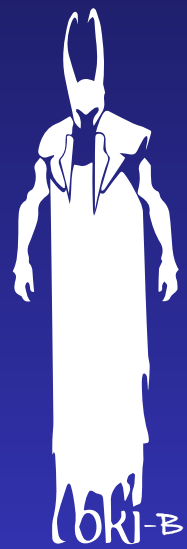
- The LisbOn KInetics (LoKI) is a simulation tool for low-temperature plasmas.
- It comprises two modules describing the electron kinetics and the ions/neutrals kinetics.

LoKI-B (open-source)

- Solves the electron Boltzmann equation
- Evaluates a prescribed electron energy distribution function

LoKI-C

- Solves a system of zero dimensional rate balance equations for the heavy particles, including transport effects



LoKI-B module

The Boltzmann equation solver

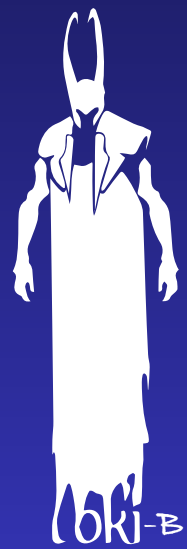
Approximations

- Non magnetised plasmas
- classical two-term expansion
- homogeneity[1]
- stationarity[1]
- no space-charge separation

Operators

- inelastic direct/stepwise and superelastic collision mechanisms with all types of excited states
- continuous approximation for rotations with Chapman-Cowling correction (CC-CAR)
- electron-electron collisions
- non-conservative ionizations

[1] Except when considering a spatial / temporal growth due to ionization



LoKI-B module

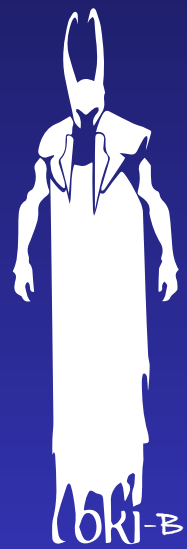
Software characteristics

Code characteristics

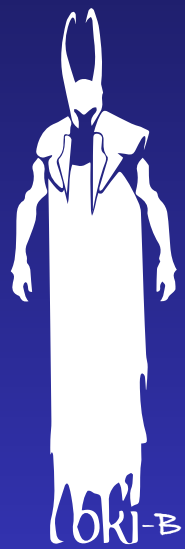
- developed under Matlab following an Object-Oriented design
- no hardcoded data (except for fundamental constants)
- user and developer friendly (easy to use / maintain / upgrade)
- handles flexible mixtures of gases / excited states

History / Status / Roadmap

- First closed beta version of LoKI-B was released early 2017 (current version **`LoKI-B_v0.6.3`**)
- Validation & Verification of the tool are currently being carried out
- Production version and public release of the tool is expected by late 2018



The code



How to use LoKI-B

Basic information about how to use the code

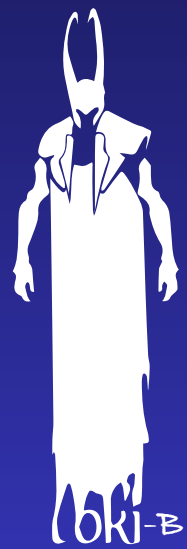
Requirements

- A PC with Matlab installed (minimum version `R2015b`)

How to use it?

- Open Matlab and navigate to the LoKI-B source folder:
  ```
  >> cd Develop/loki/Code
  ```
- Issue the command:
  ```
  >> loki('setup_file.in')
  ```
- The main User Interface (UI) is the "setup file".

The question is: How to configure the setup file?



The “setup file” at a glance

Structure of the setup file

The setup file

- Located in the `Input` folder
- Plain text file (“`.in`” extension just for organisation purposes)
- Comment character: `%`
- Indentation structured blocks
- Five sections:
  - `workingConditions`
  - `electronKinetics`
  - `chemistry`
  - `gui`
  - `output`

NOTE: a full GUI is on the roadmap. Right now the GUI is only for output purposes.

```
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%   DEFAULT CONFIGURATION FILE LOKI-B    %
% (subject to change during development) %
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%

% --- configuration of the working conditions ---
workingConditions:
  gasPressure: 133.32                          % in Pa
  gasTemperature: 300                          % in K
  electronDensity: 9.8e9                       % in m-3
  electronTemperature: linspace(0.03,5,50)     % in eV
  chamberLength: 1.0                           % in m
  chamberRadius: 1.0                           % in m
  reducedField: logspace(-2,1,50)              % in Td
  excitationFrequency: 0                       % in Hz

% --- configuration of the electron kinetics ---
electronKinetics:
  isOn: true              % true or false
  eedfType: boltzmann     % boltzmann or maxwellian
%  CARgases: N2           % gases for which CAR is on
  LXCatFiles:             % cross section files
    - N2_LXCat.txt
    - N2_rot_LXCat.txt
%  LXCatFilesExtra: extra_LXCat.txt    % extra cross section files
%  effectiveCrossSectionPopulations:   % see doc
%    - N2_effectivePop.txt
  gasProperties:         % properties of the gases
    mass: databaseMasses.txt
    fraction:
      - N2 = 1
    harmonicFrequency: databaseHarmonicFrequencies.txt
    anharmonicFrequency: databaseAnharmonicFrequencies.txt
    rotationalConstant: databaseRotationalConstants.txt
    electricQuadrupoleMoment: databaseQuadrupoleMoment.txt
  stateProperties:       % properties of the states
    energy:
      - N2(X,v=*) = harmonicOscillatorEnergy
      - N2(X,v=0,J=*) = rigidRotorEnergy
    statisticalWeight:
      - N2(X,v=*) = 1.0
      - N2(X,v=0,J=*) = rotationalDegeneracy_N2
    population:
      - N2(X) = 1.0
      - N2_vibpop.txt
      - N2(X,v=0,J=*) = boltzmannPopulation@gasTemperature
  energyGrid:            % properties of the energy grid
    maxEnergy: 1
    cellNumber: 1000
    smartGrid:           % configuration of the smart grid
      minEedfDecay: 20
      maxEedfDecay: 25
      updateFactor: 0.05

% --- configuration for the heavy species kinetics ---
chemistry:
  isOn: false

% --- configuration of the grafical user interface ---
gui:
  isOn: true
  refreshFrequency: 2

% ---  configuration of the output files ---
output:
  isOn: false
  folder: simulation1
  dataFiles:
    - eedf
    - swarmParameters
    - rateCoefficients
    - powerBalance
    - lookUpTable
```

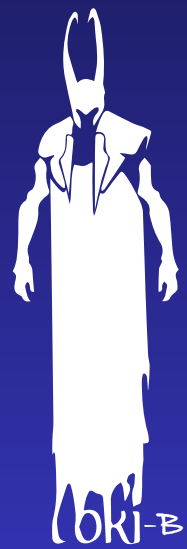
LoKI-B Input

Information required by the code

Information provided / selected by the user

The user must provide three types of information

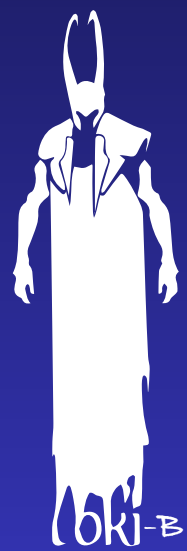
- Information about physical parameters
  - working conditions
  - collisional data (http://www.lxcat.net)
  - atomic and molecular data
  - species populations
- Information about physical models
  - e-e collisions
  - electron density growth model
  - energy sharing mode in ionization collisions
- Information about numerical details
  - energy grid



LoKI-B Output

Information returned by the code

Parameter	Expression
Reduced free diffusion coefficient	$D_e N = \frac{2e}{3m_e}\int_0^\infty \frac{u^{3/2}}{\nu_c/N} f(u)du$
Reduced mobility	$\mu_e N = -\frac{2e}{3m_e}\int_0^\infty \frac{u^{3/2}}{\nu_c/N}\frac{df(u)}{du}du$
Electron drift velocity	$v_d = \mu_e E$
Characteristic energy	$u_{\text{Char}} = \frac{D_e}{\mu_e}$
Mean energy	$\varepsilon = \int_0^\infty u^{3/2} f(u)du$
Electron “temperature”	$T_e = \frac{2}{3}\varepsilon$
Electron impact rate coefficients	$C_{i,j} = \sqrt{\frac{2e}{m_e}}\int_0^\infty \sigma_{i,j} u f(u)du$
Reduced Townsend coefficient	$\frac{\alpha}{N} = \frac{C_I}{v_d}$



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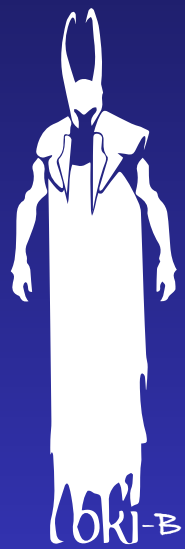
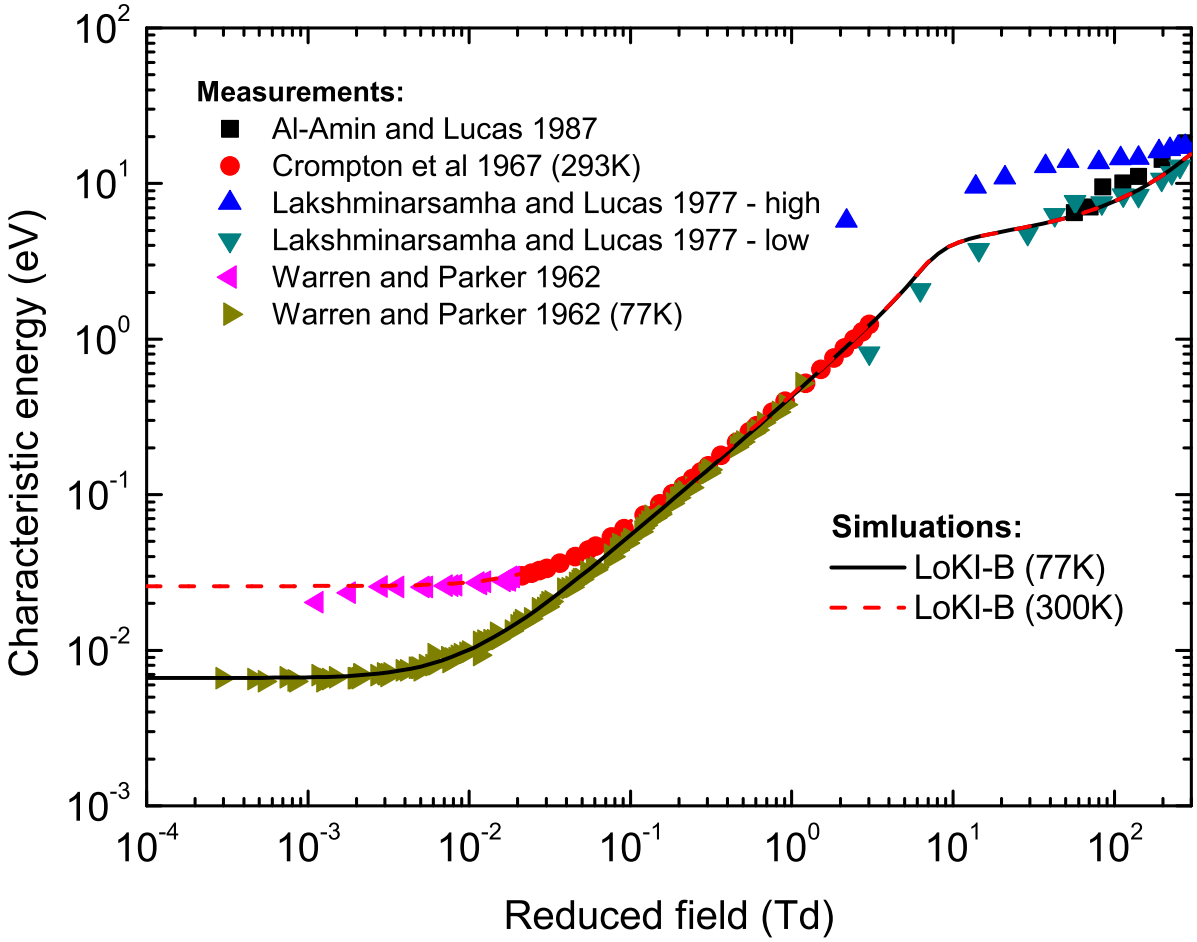


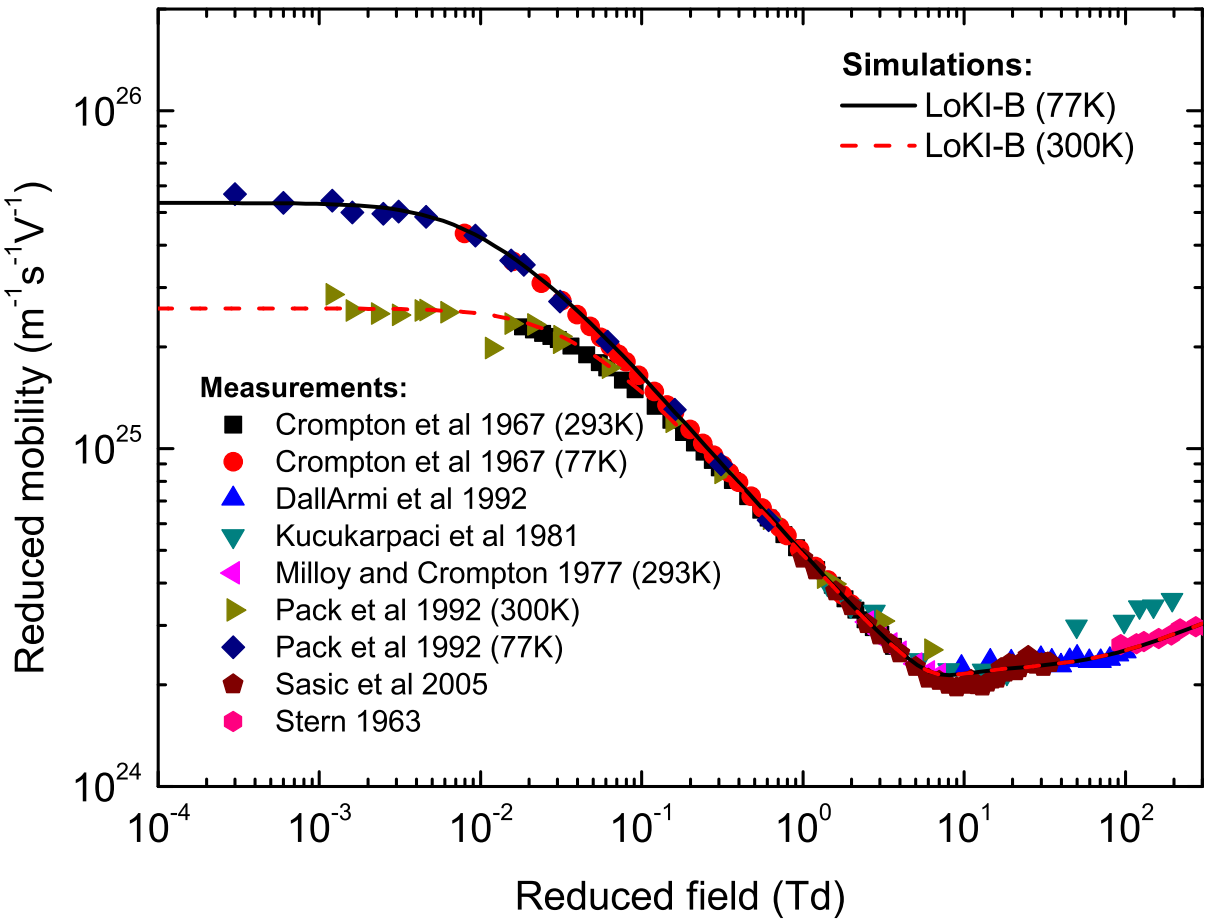
Swarm analysis of He

Characteristic energy



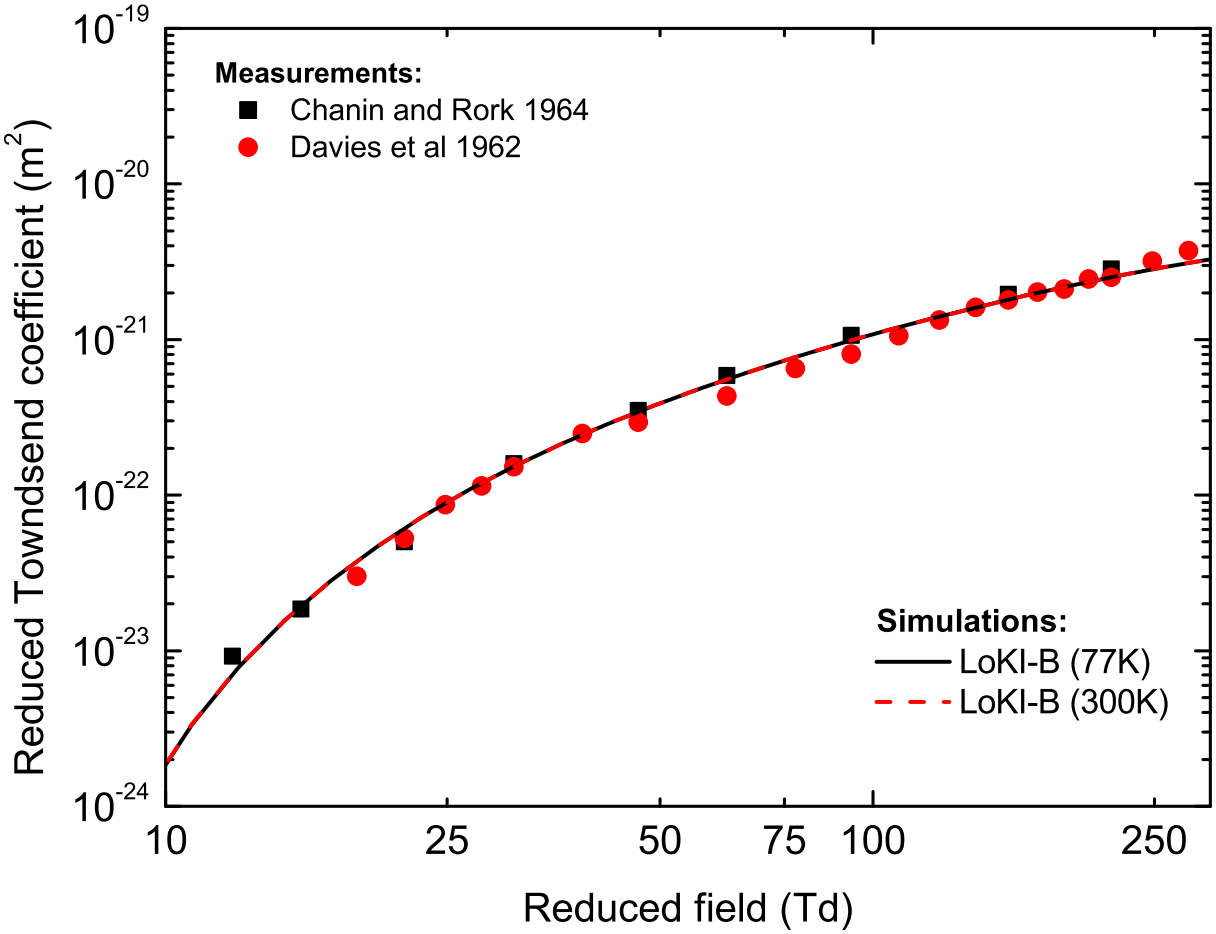
Swarm analysis of He

Reduced mobility



Swarm analysis of He

Reduced Towndsend coefficient



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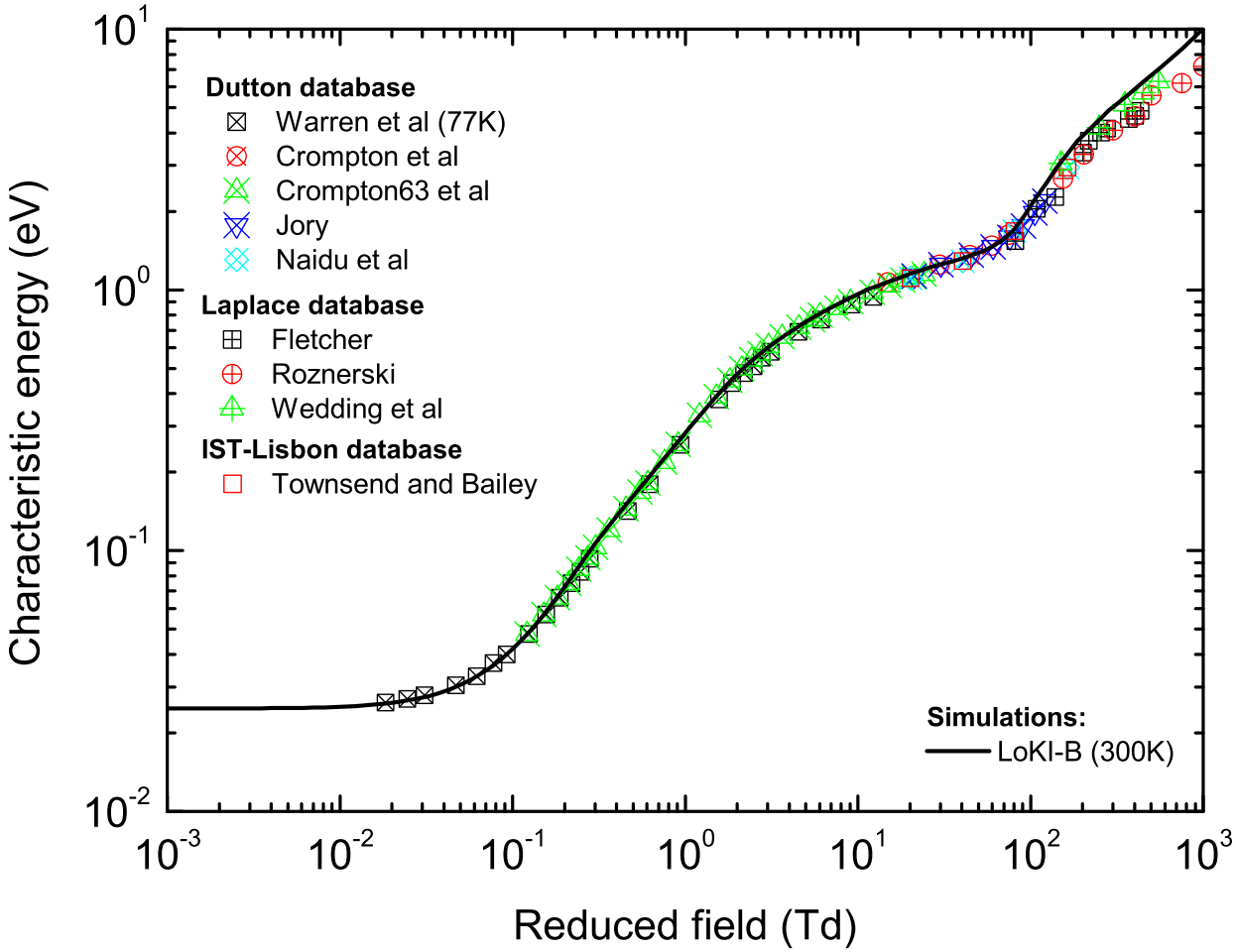
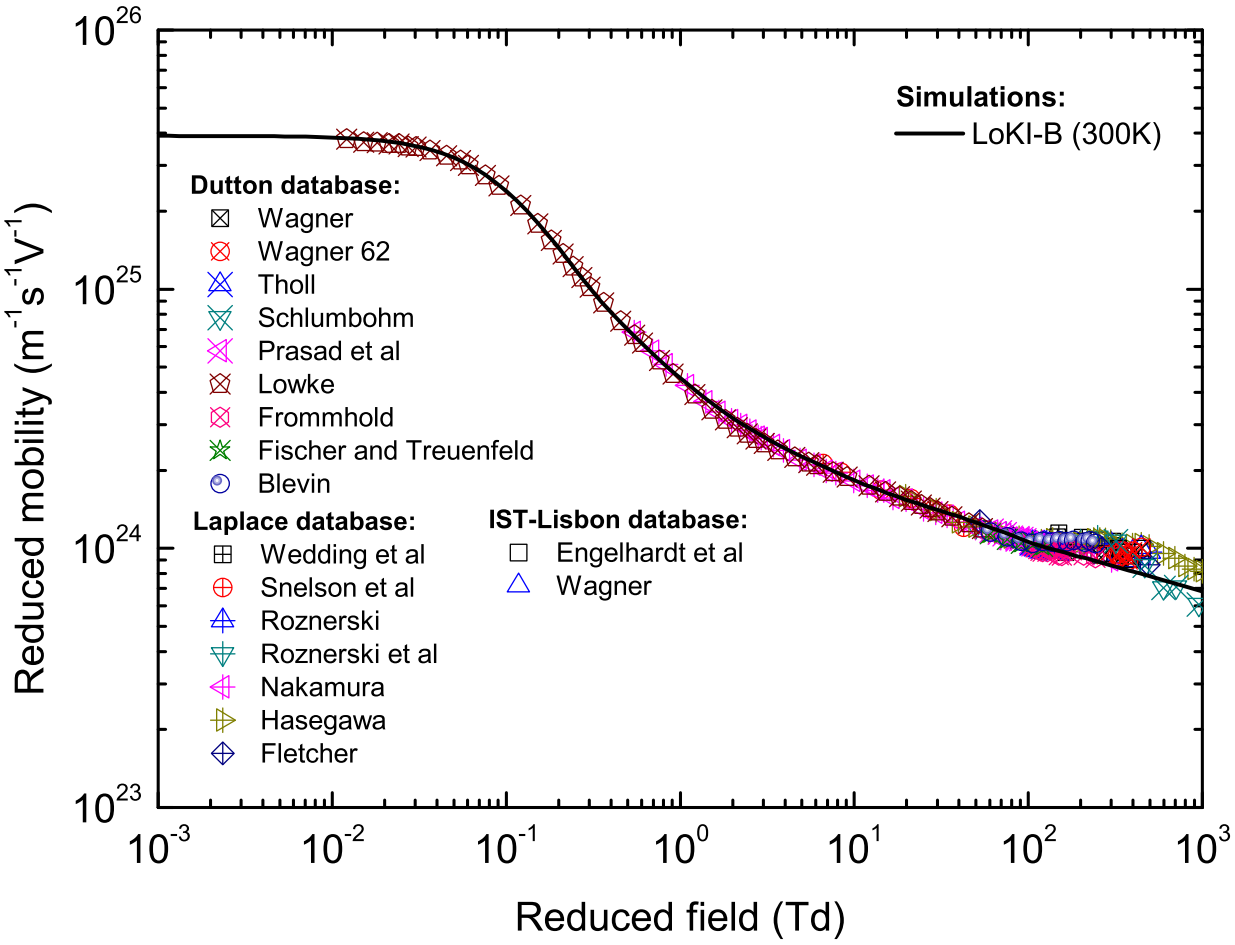


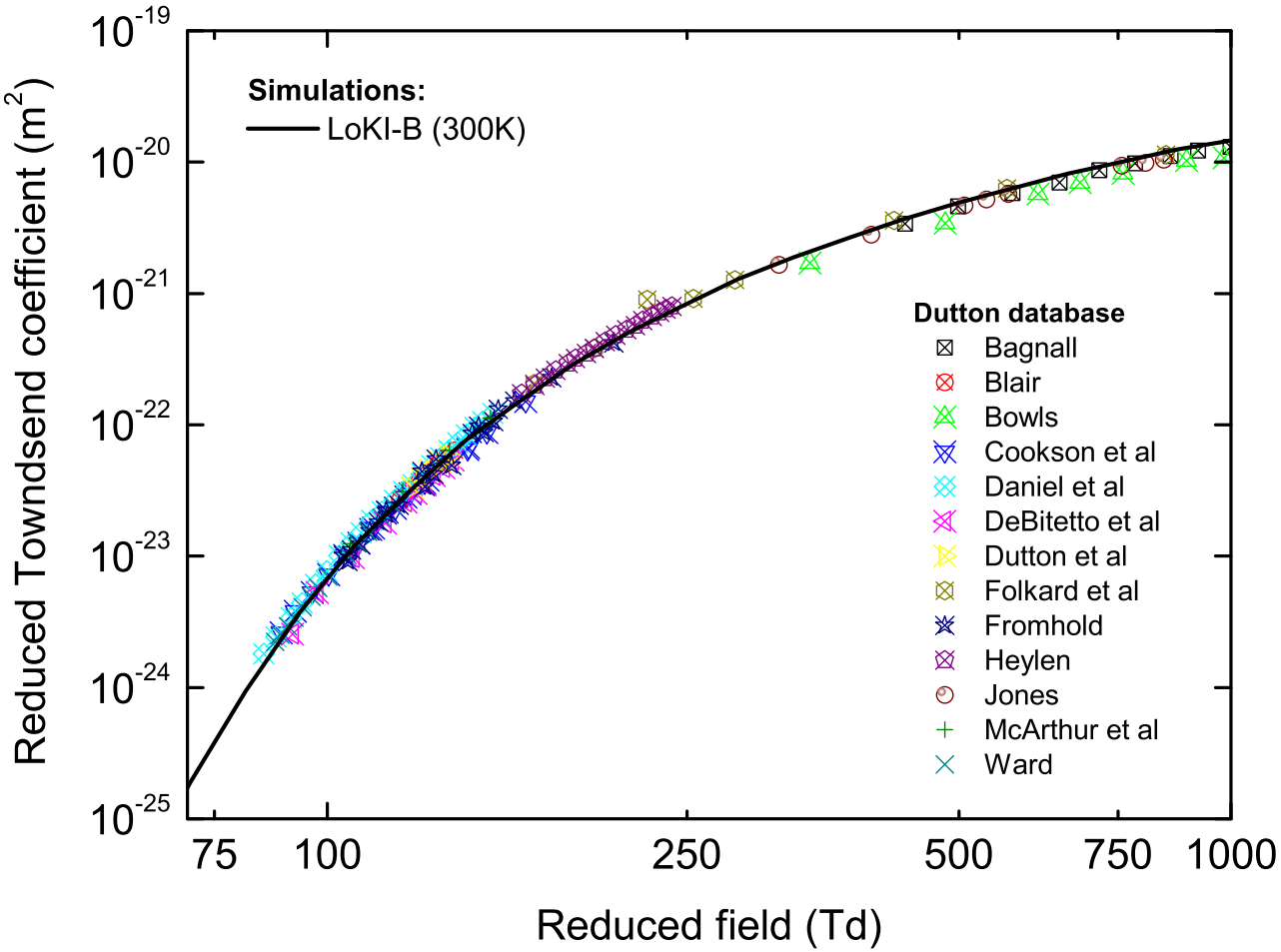
Swarm analysis of N_2

Reduced mobility



Swarm analysis of N_2

Reduced Towndsend coefficient



Thank's for your attention!

Contact information:
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