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Sticking and Re-erosion of C_xH_y Molecules

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Introduction

- Chemical sputtering of carbon by hydrogen produces volatile hydrocarbon species (C_xH_y)
- These C_xH_y species are transported through the plasma boundary layer
- Neutral C_xH_y species are not confined by the magnetic field and can be transported to remote areas
- Redeposition of hydrocarbon films due to long range transport of C_xH_y species with low surface loss probability
- Investigation of neutral, low-energy radicals in laboratory plasmas (next slide)
- Ionisation in the boundary layer produces energetic C_xH_y species. Little is known about their interaction with the surface (reflection and sticking data)
- Important input data for modelling of transport in the boundary plasma

→ Experimental and theoretical attempt to determine reflection and sticking coefficients of different C_xH_y species

→ MD results

Sticking of thermal neutrals

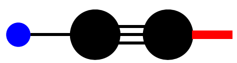
Experiment:
determination of the surface loss probability β of different hydrocarbon radicals in low-temperature plasmas using cavity probes
Result:

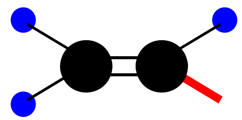
➔ 3 different β values are necessary and sufficient

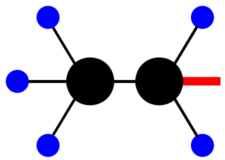
➔ 3 different types of growth precursors

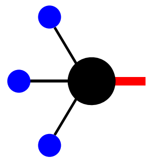
interpretation: β depends mainly on the hybridisation state of the carbon atom carrying the dangling bond

sp¹	sp²	sp³
C_2H	C_2H_3	C_2H_5 or CH_3









$\beta \approx 0.8$	$\beta \approx 0.3$	$\beta < 10^{-2}$

C. Hopf, T. Schwarz-Selinger, W. Jacob, and A. von Keudell: “Surface Loss Probabilities of Hydrocarbon Radicals on Amorphous Hydrogenated Carbon Film Surfaces”, Journal of Applied Physics 87, 2719–2725 (2000).

Theoretical description

TRIM (binary collision approximation):

- applicable at high energies ($E_{ion} > 50$ eV)
- fast
- can not treat molecular effects

Molecular dynamics (solution of equation of motion):

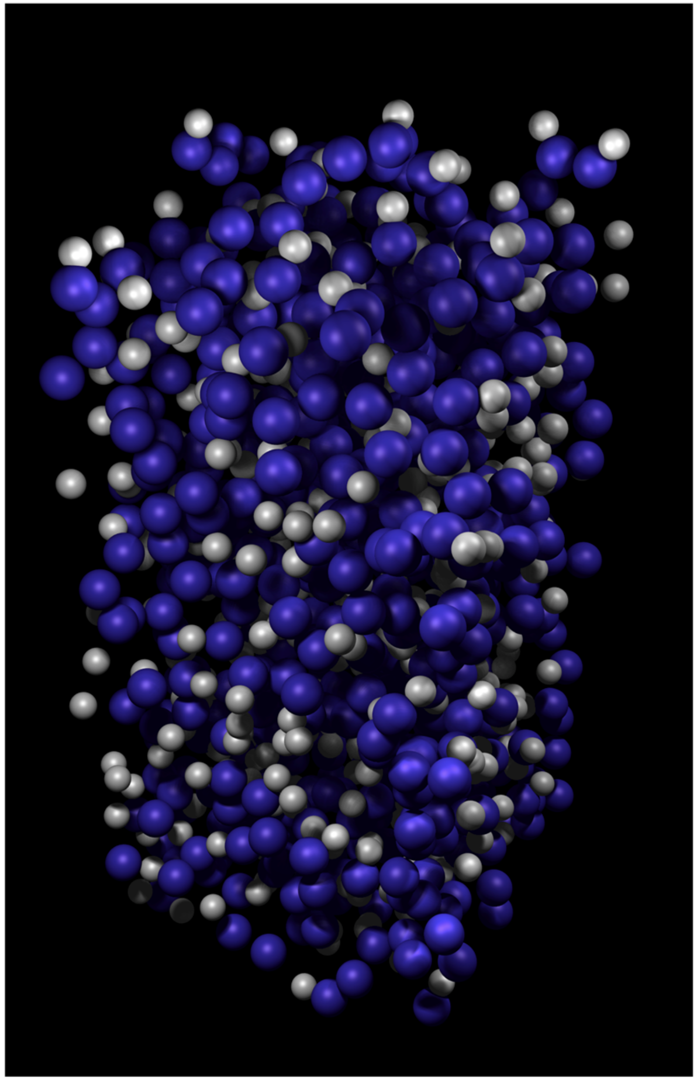
- applicable at low energies ($E_{ion} < 100$ eV)
- slow (computation time intensive)
- can treat molecular effects

- **But quality of results depends on quality of used interaction potential**
- **Experimental verification of (some) results highly desirable**

MD sample (amorphous hydrogenated carbon, a-C:H)

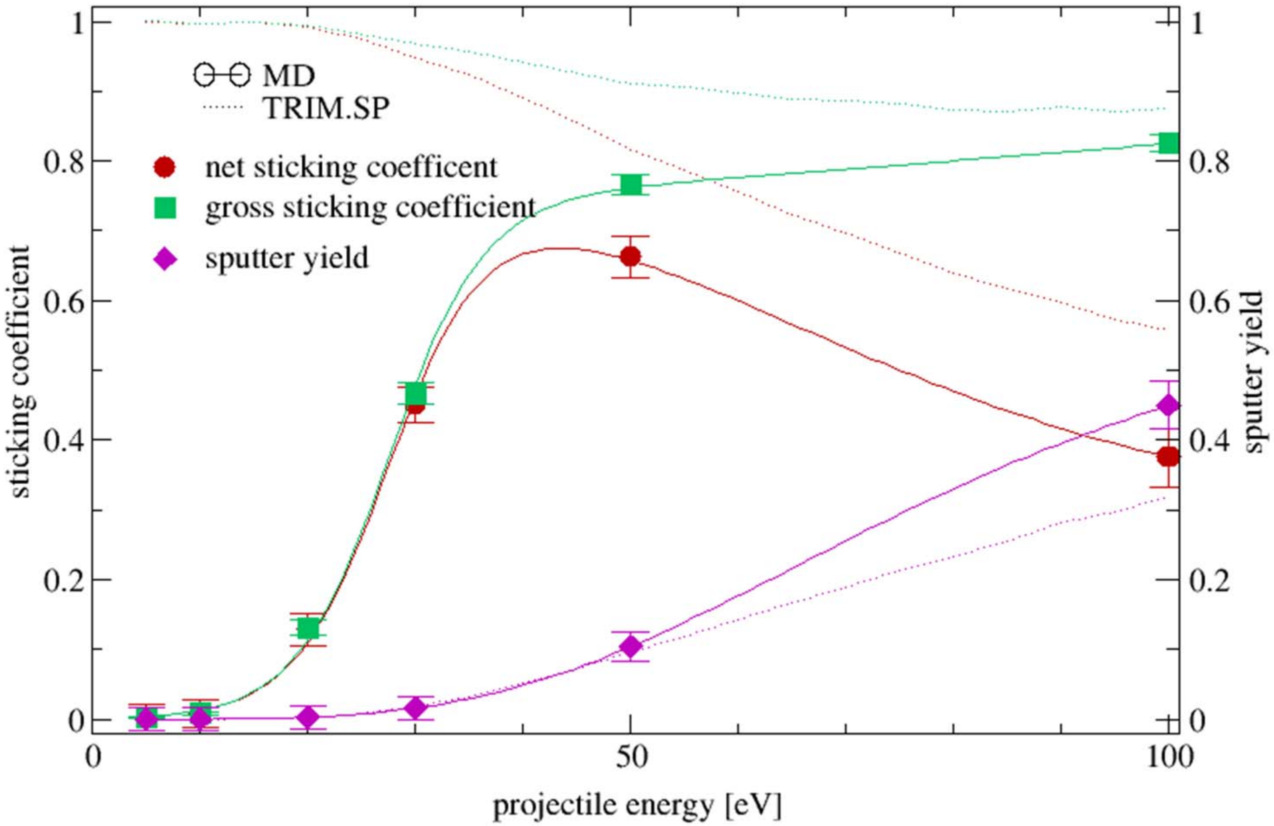
- 986 Atoms
  - 592 Carbon
  - 384 Hydrogen / Deuterium
- 14 Å x 14 Å x 30 Å

- Production:
  - Random placement of atoms
  - multiple annealing cycles



P. N. Maya, U. von Toussaint, and C. Hopf:
Synergistic erosion process of hydrocarbon films:
A molecular dynamics study.
New J. Phys., ***10***, *023002 (15pp), 2008.*

Sticking of CH_4: TRIM vs. MD



Symbols
= MD results

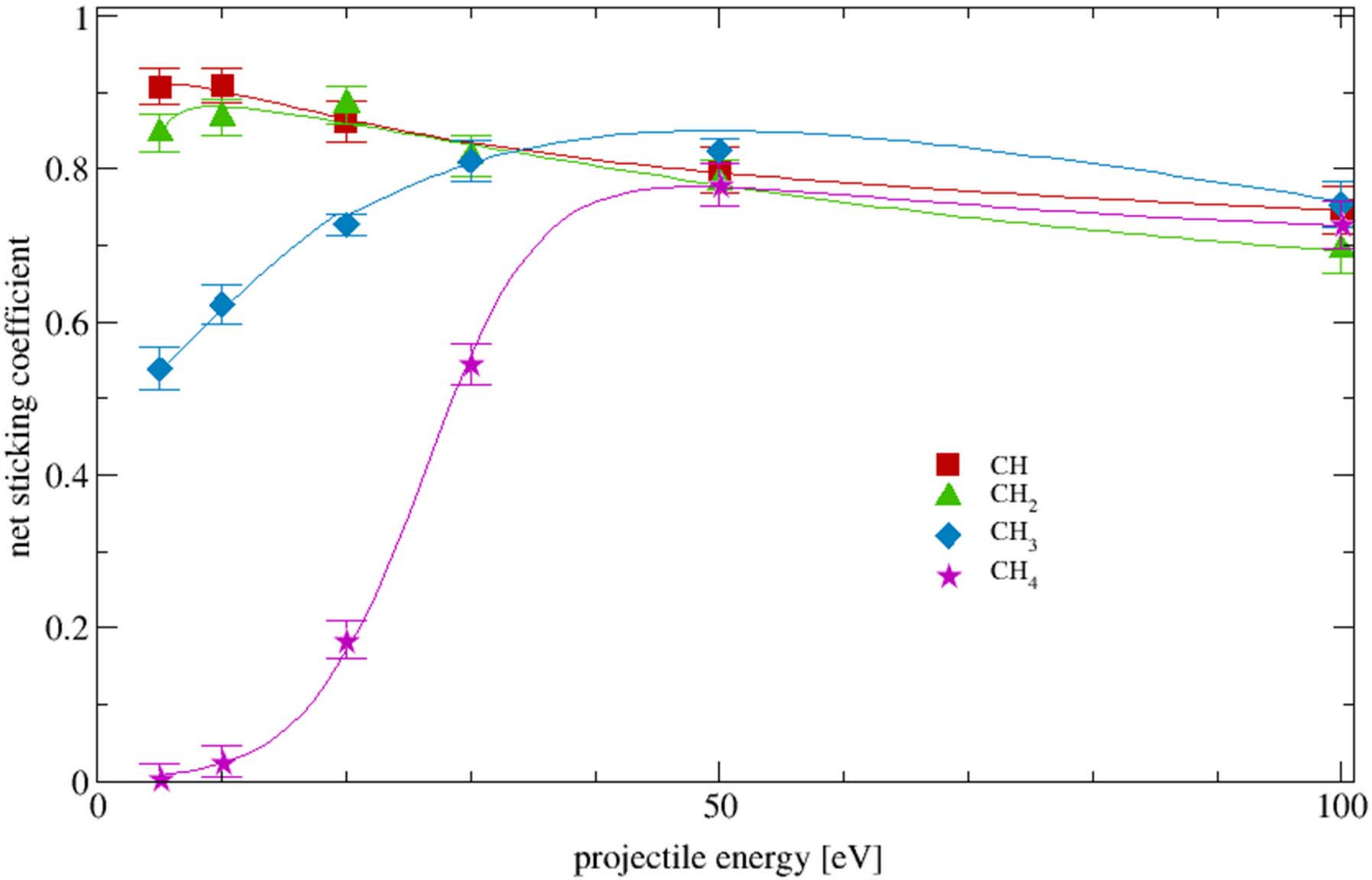
Solid lines
= fit through MD results

Dashed lines
= TRIM.SP results

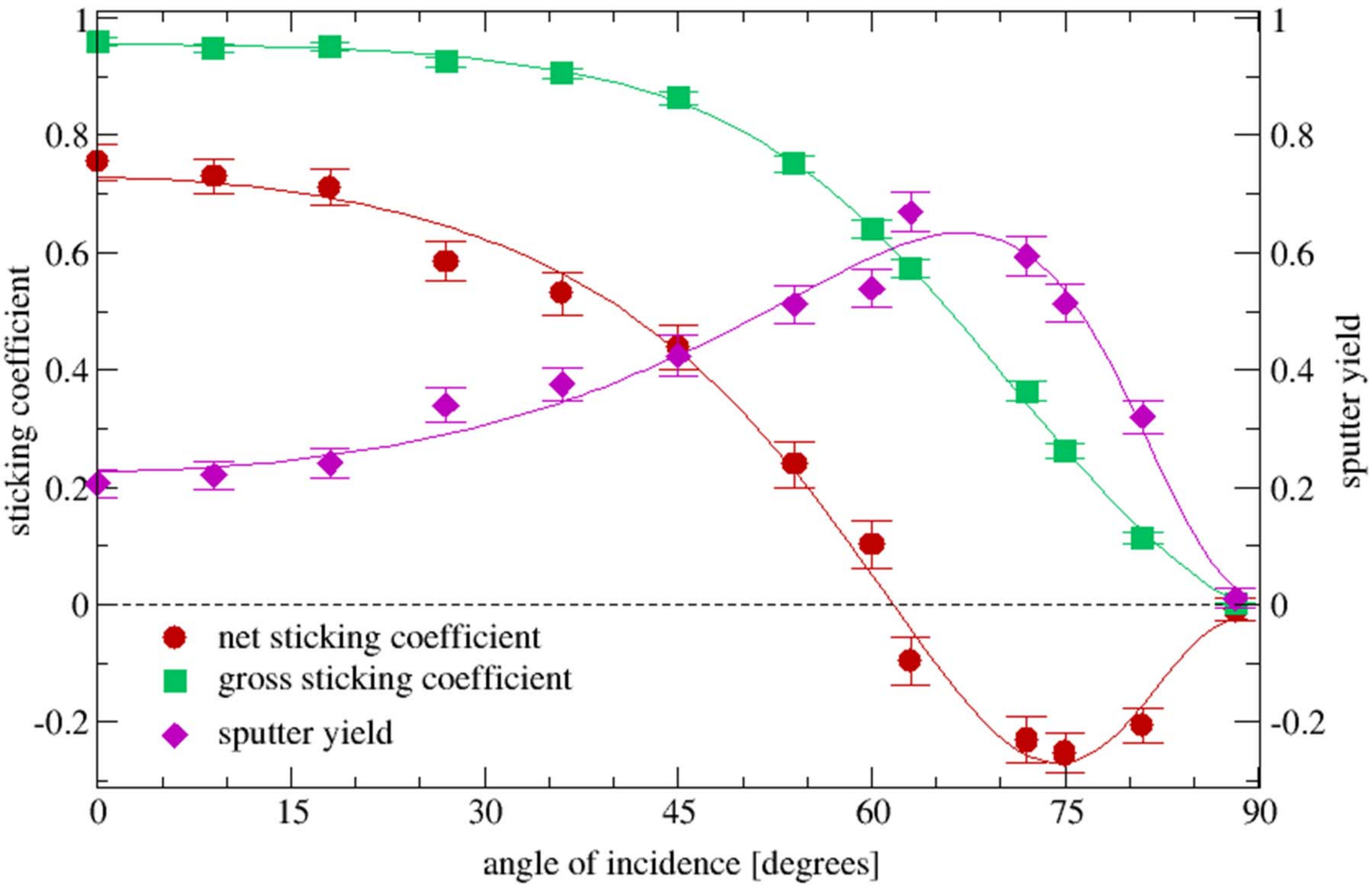
Threshold energy for sticking
TRIM results comparable at high energies
TRIM yields wrong trend at low energies

Sticking of different CH_y species: Energy dependence

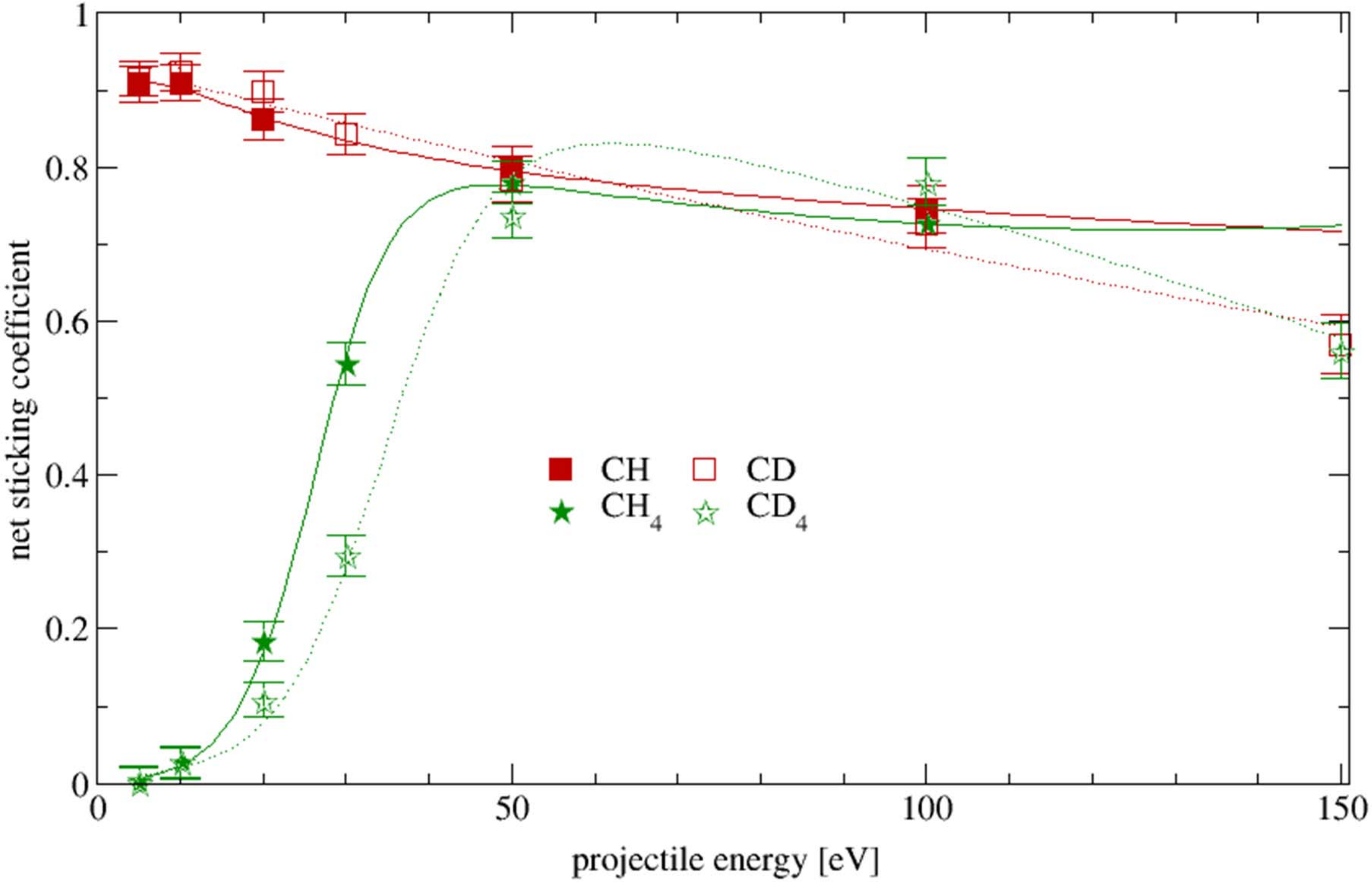
perpendicular incidence



Sticking of CH_3 (100 eV): Angle dependence



Sticking of different CH_y species: Isotope effect



Fit formulae

Angle dependence

$$Y(E_0,\theta_0) = Y(E_0,0)\left\{\cos\left[\left(\frac{\theta_0}{\theta_0^*}\frac{\pi}{2}\right)^c\right]\right\}^{-f}\times$$
$$\exp\left(b\left\{1-1/\cos\left[\left(\frac{\theta_0}{\theta_0^*}\frac{\pi}{2}\right)^c\right]\right\}\right)$$

$$\theta_0^* = \pi - \arccos\sqrt{\frac{1}{1+E_0/E_{sp}}}.$$

	E_0[eV]	$Y(0)$	E_{sp}[eV]	f	b	c
CH_4	20	0.00152	2.8	20.1	14.8	0.492
	30	0.0306	2.8	-2.76	-0.447	1.13
	50	0.0799	2.8	3.19	1.84	1.23
	100	0.213	2.8	6.36	3.46	0.914
CH_3	20	0.0118	2.8	8.7	5.72	0.957
	30	0.0433	2.8	3.71	2.34	1.07
	50	0.106	2.8	3.09	1.44	1.19
	100	0.227	2.8	5.1	2.51	0.966
CH_2	20	0.0316	2.8	7.08	4.4	1.1
	30	0.0879	2.8	1.66	0.852	1.35
	50	0.145	2.8	3.46	1.63	1.13
	100	0.264	2.8	4.9	2.37	0.96
CH	10	0.0143	2.8	7.36	4.71	1.52
	20	0.0566	2.8	3.91	2.22	1.17
	50	0.129	2.8	5.23	2.53	0.966
	100	0.221	2.8	6.5	3.19	0.841
C	10	0.0105	2.8	7.75	4.4	2.17
	20	0.0501	2.8	2.96	1.62	1.28
	50	0.139	2.8	3.99	1.76	1.08
	100	0.236	2.8	5.9	2.76	0.886

K. Tichmann, U. von Toussaint, T. Schwarz-Selinger, and W. Jacob:
"Determination of the Sticking Probability of Hydrocarbons on an Amorphous Hydrocarbon Surface"
Physica Scripta T138, 014015 (4pp) (2009).

K. Tichmann, U. von Toussaint, T. Schwarz-Selinger, and W. Jacob:
"Measurement and Modeling of Reflection and Sticking Probabilities of Energetic Hydrocarbon Species"
Journal of Nuclear Materials, accepted (2010) (PSI-Proceedings).

Summary

- Sticking and reflection of C_xH_y was simulated by MD
- Energy dependence
- Angle dependence
- Species dependence
- Isotope effect
- Simulated data were fitted by empirical fit functions
- Complete set of data is available

END