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# Impact of Organic Carbon on Soot Light Absorption

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PTL Particle Technology Laboratory

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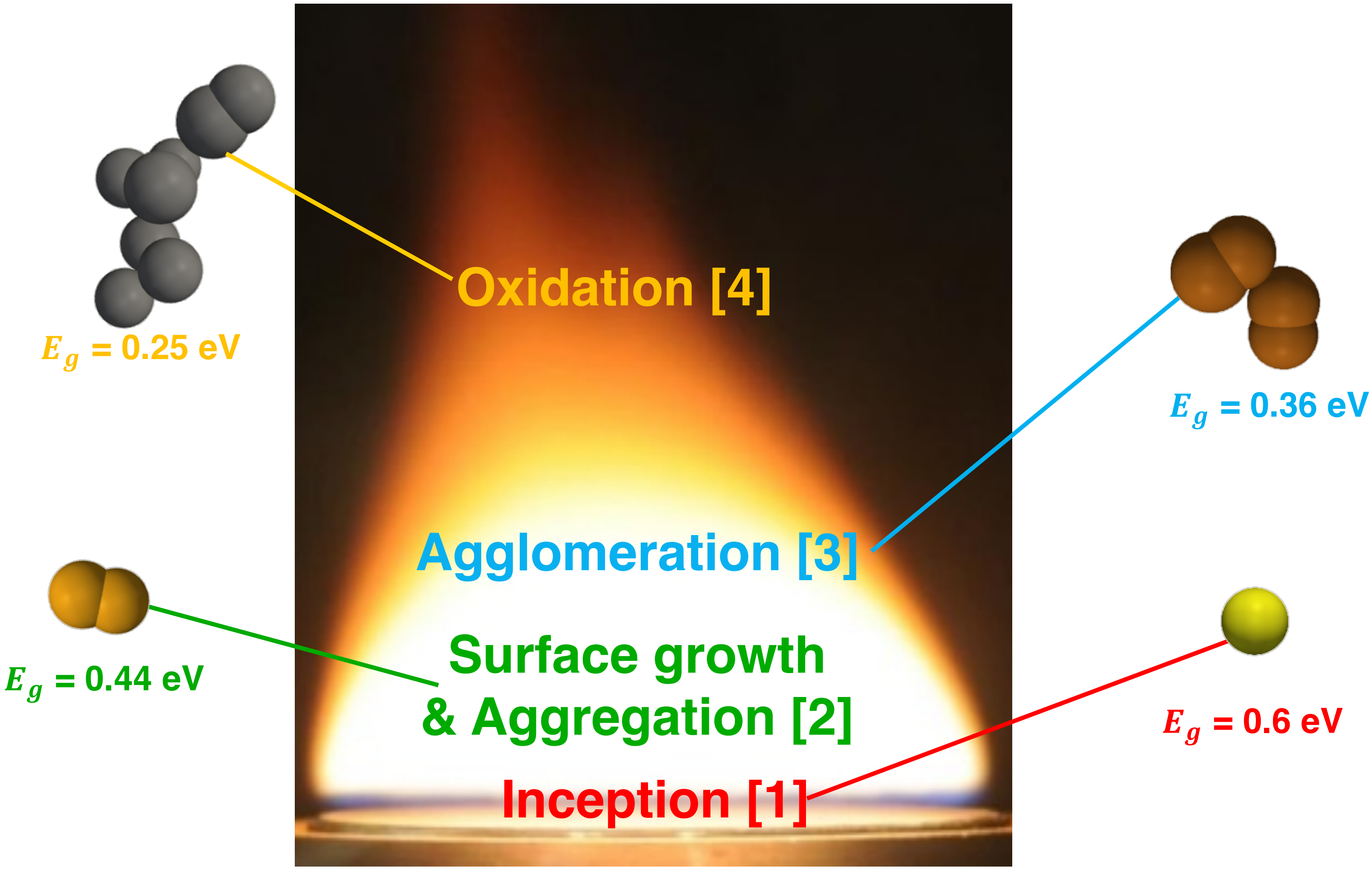
# Soot dynamics in fuel-rich flames





[4] G.A. Kelesidis, S.E. Pratsinis, *Combust. Flame* **209** (2019) 493.
[3] G.A. Kelesidis, E. Goudeli, S.E. Pratsinis, *Carbon* **121** (2017) 527.
[2] G.A. Kelesidis, E. Goudeli, S.E. Pratsinis, *Proc. Combust. Inst.* **36** (2017) 29.
[1] M.R. Kholghy, G.A. Kelesidis, S.E. Pratsinis, *Phys. Chem. Chem. Phys.* **20** (2018) 10926.

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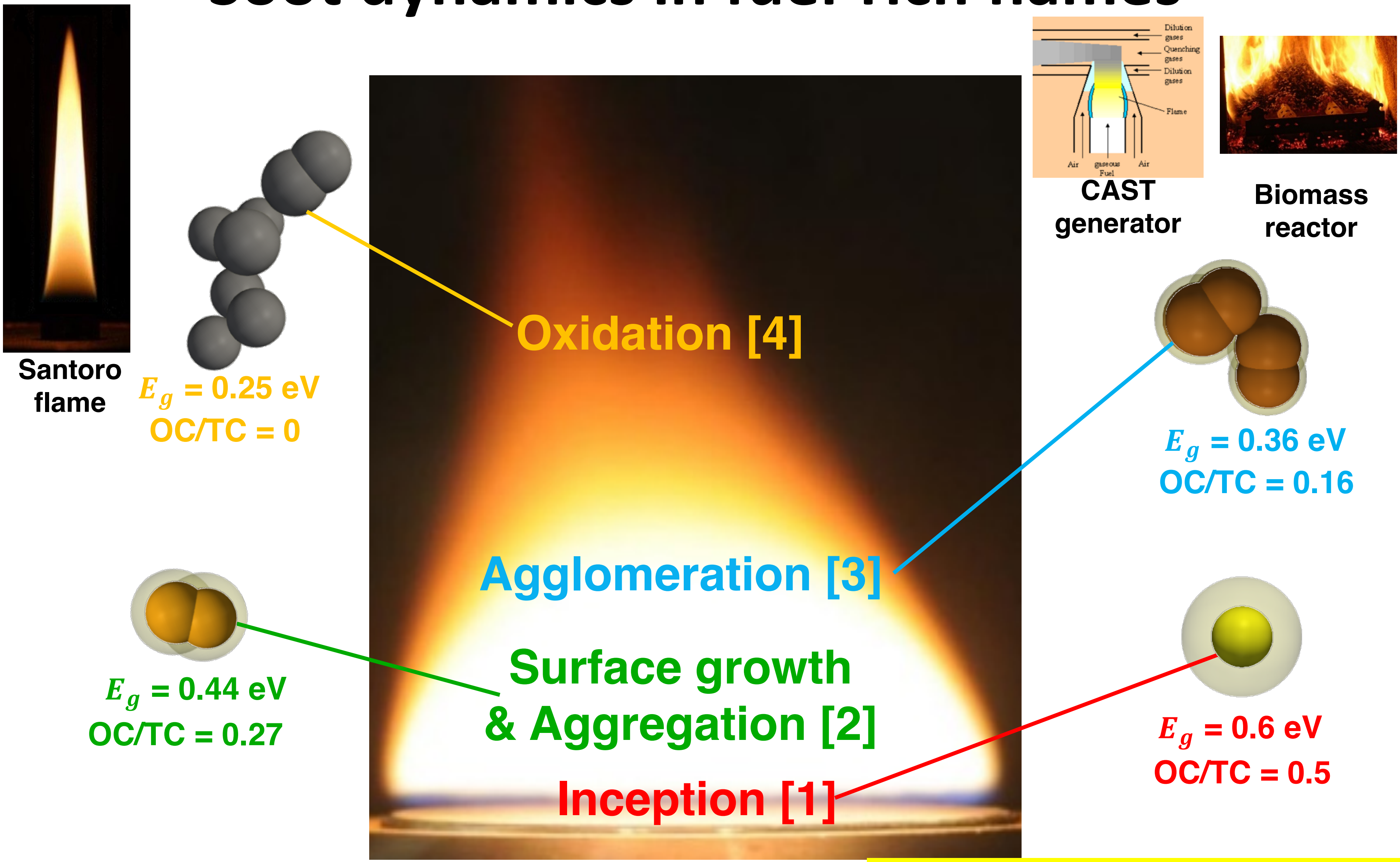


**Organic Carbon (OC): Volatile & Semi-volatile organic compounds**


[4] G.A. Kelesidis, S.E. Pratsinis, *Combust. Flame* **209** (2019) 493.
[3] G.A. Kelesidis, E. Goudeli, S.E. Pratsinis, *Carbon* **121** (2017) 527.
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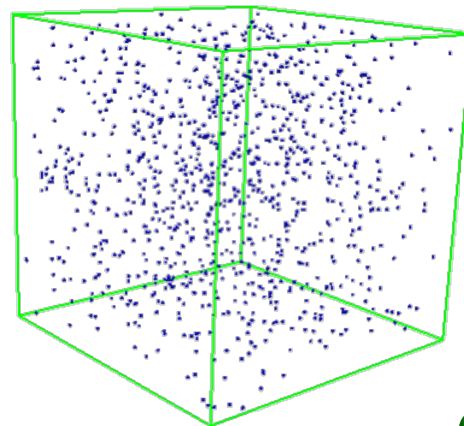
# Soot Dynamics by Discrete Element Modeling (DEM)

i) Initial configuration inception has largely ended.



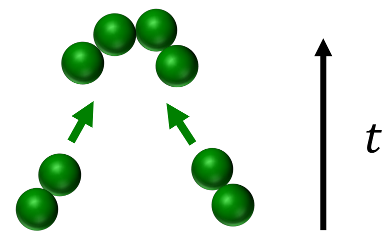
$T$ = 1830 K

$d_{m,o}$ = 2 nm

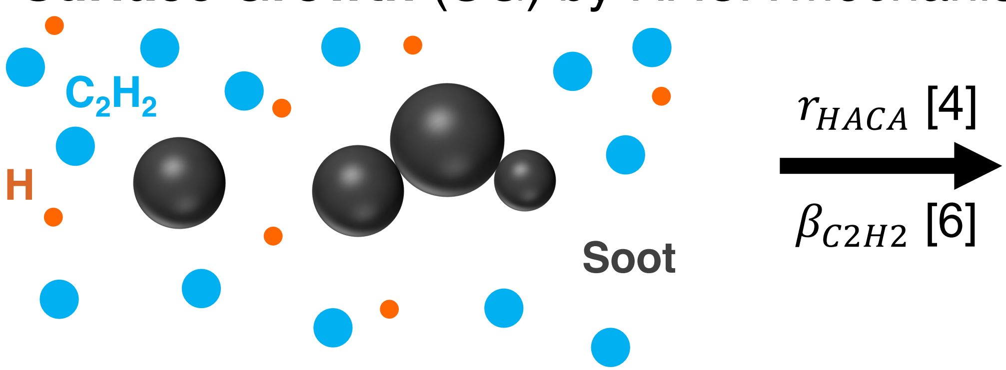
$N_{tot,o}$ = 4.5·10$^{16}$ m$^{-3}$

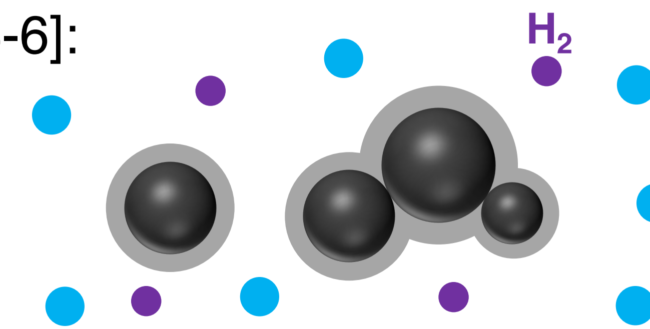
[1,2]

ii) Discrete Element Modeling (DEM) of **Particle Motion** and **Agglomeration** [3]




iii) **Surface Growth** (SG) by HACA mechanism [4-6]:




Mass Balance for each $C_2H_2$ reaction:

$$\pi \frac{d^3_{p,new}}{6} \rho_{soot} = \pi \frac{d^3_{p,old}}{6} \rho_{soot} + m_{2c}$$


[1] Abid, A. D.; Heinz, N.; Tolmachoff, E.D.; Phares, D.J.; Campbell, C.S.; Wang, H. Combust Flame 2008, 154, 775.

[2] Camacho ,J.; Liu, C.; Gu, C.; Lin, H.; Huang, Z.; Tang, Q.; You, X.; Saggese, C.; Li, Y.; Jung, H.; Deng, L.; Wlokas, I.; Wang, H. Combust Flame 2015, 162, 3810.

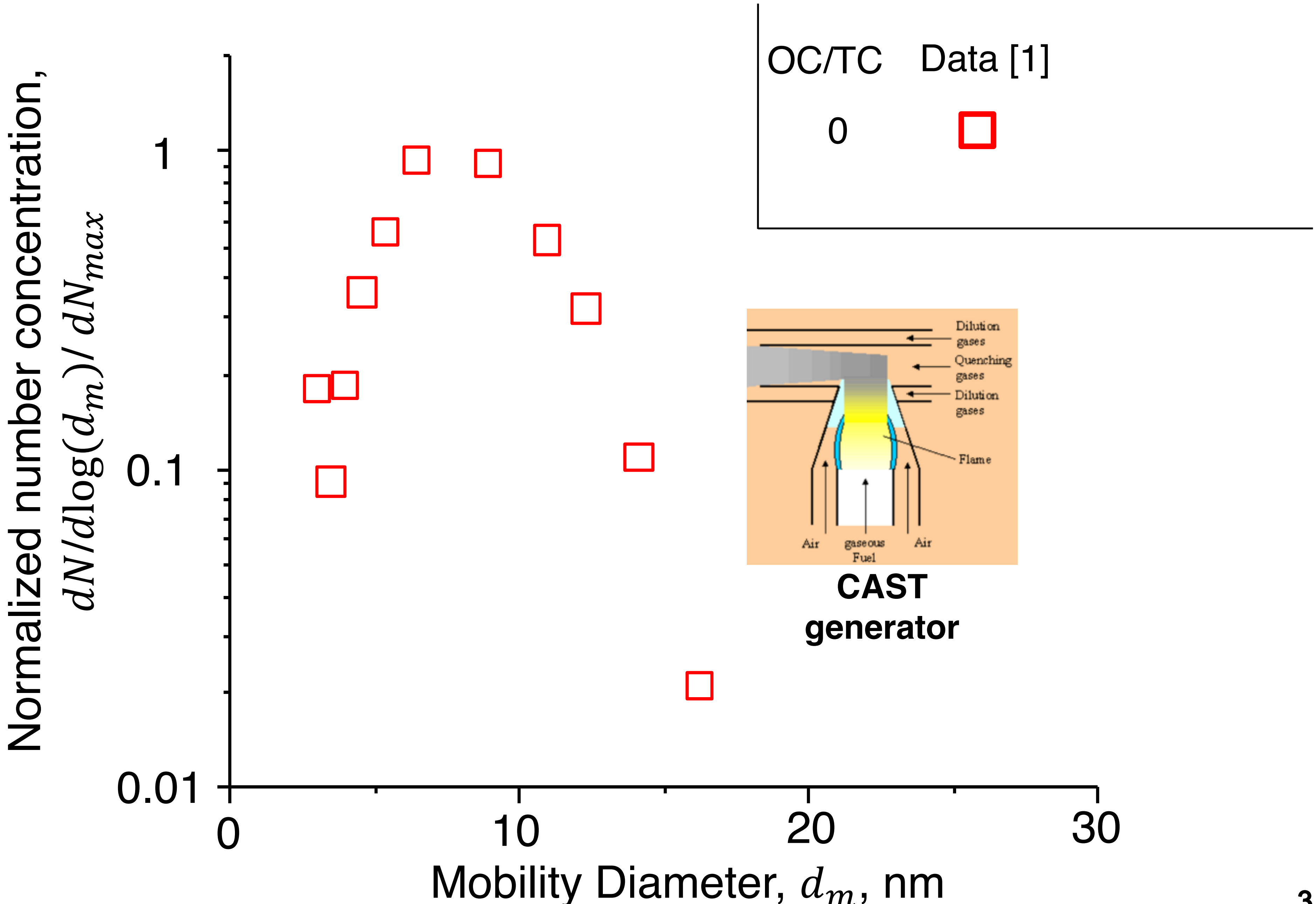
[3] Goudeli, E.; Eggersdorfer, M. L.; Pratsinis, S. E. Langmuir 2015, 31,1320.

[4] Appel, J.; Bockhorn, H.; Frenklach, M. Combust Flame 2000, 121, 122.

[5] Saggese, C.; Ferrario, S.; Camacho, J.; Cuoci, A.; Frassoldati, A.; Ranzi, E.; Wang, H.; Faravelli, T. Combust Flame 2015, 162, 3356.

**[6] Kelesidis, G. A.; Goudeli, E.; Pratsinis, S. E. Proc Combust Inst 2017 36, 29.**

# Validation of soot size distribution




**CAST generator**


[1] Maricq, M.M., *Aerosol Sci. Technol.* **48** (2014) 620.

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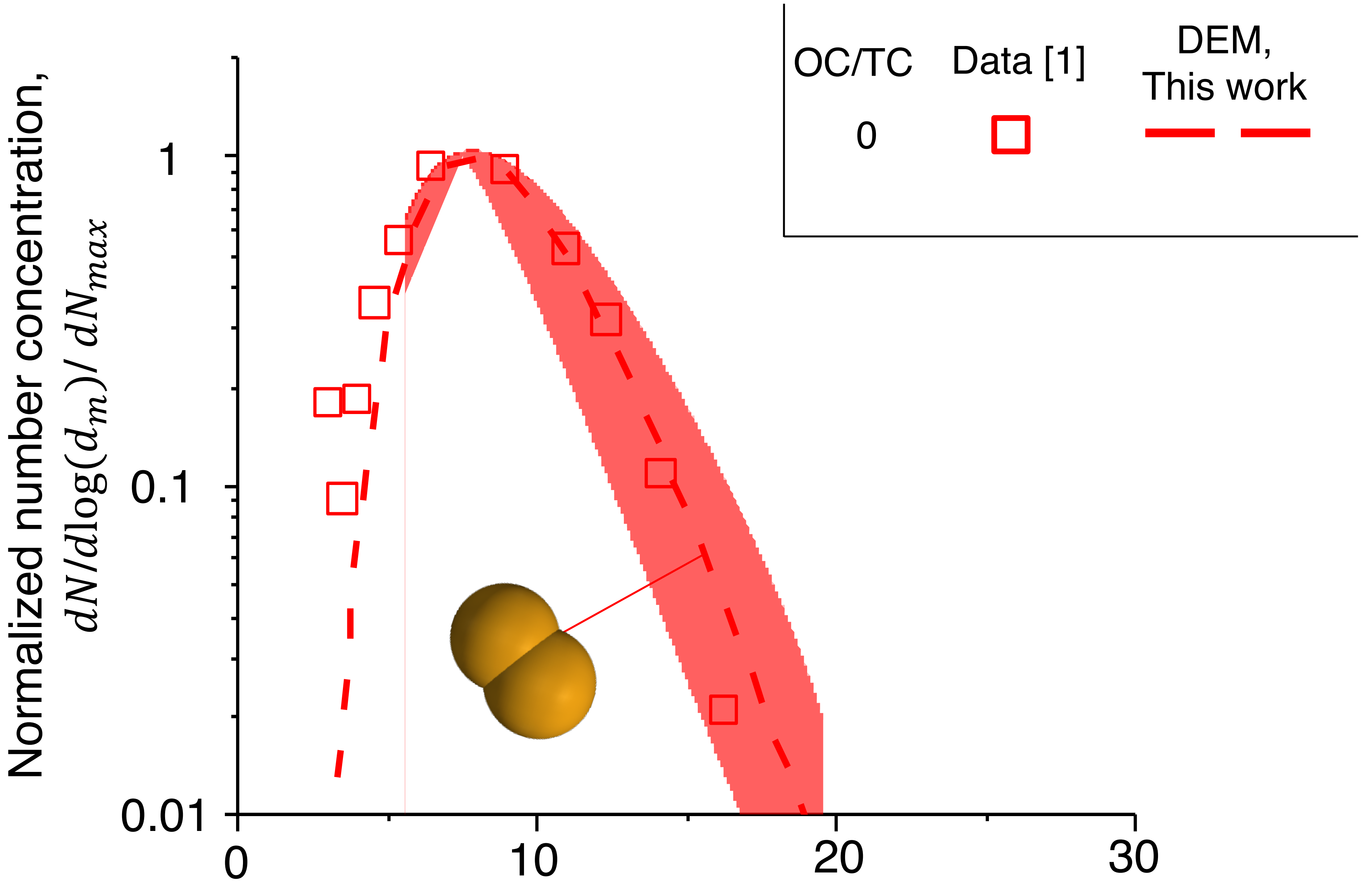


[1] Maricq, M.M., *Aerosol Sci. Technol.* **48** (2014) 620.

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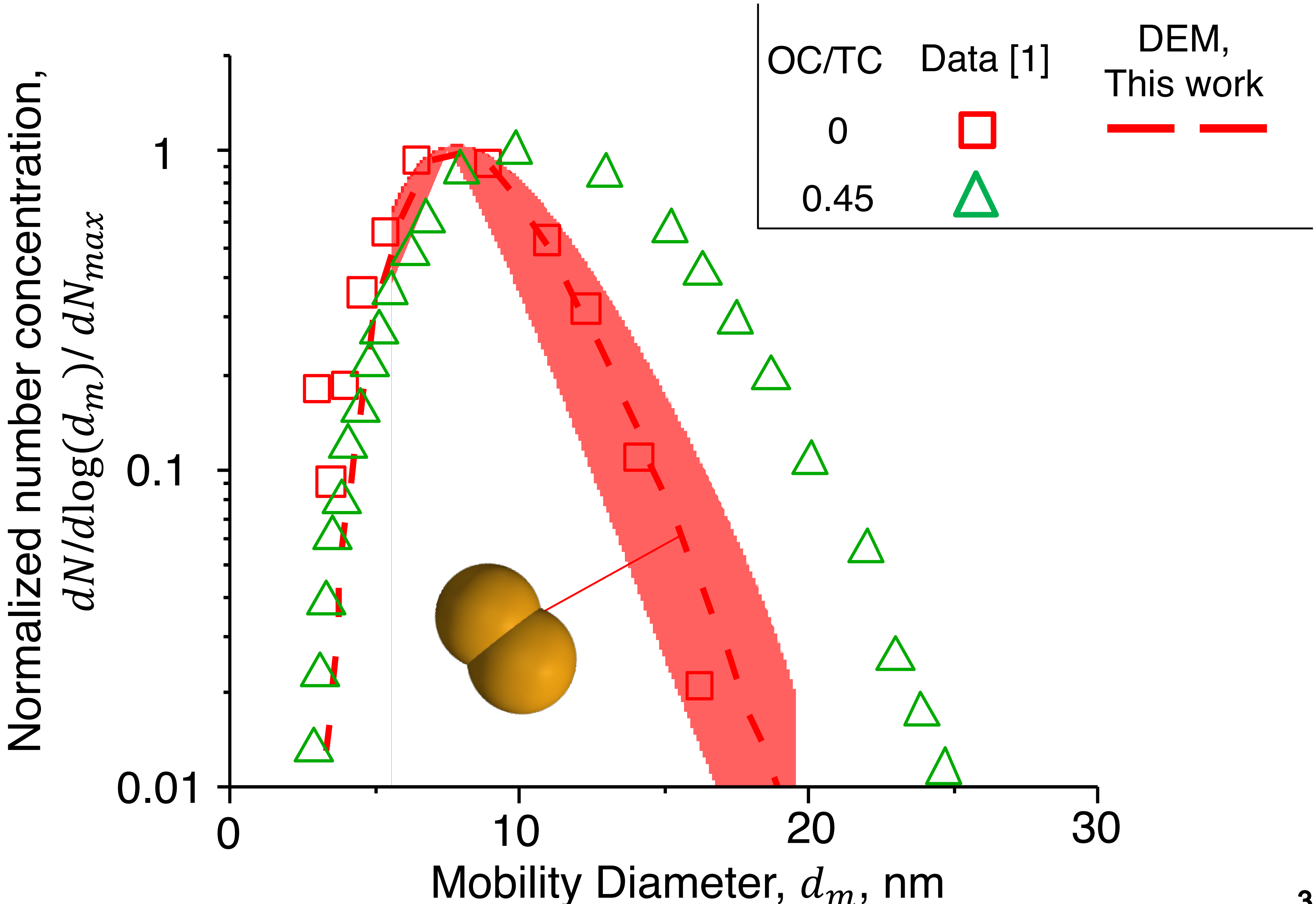




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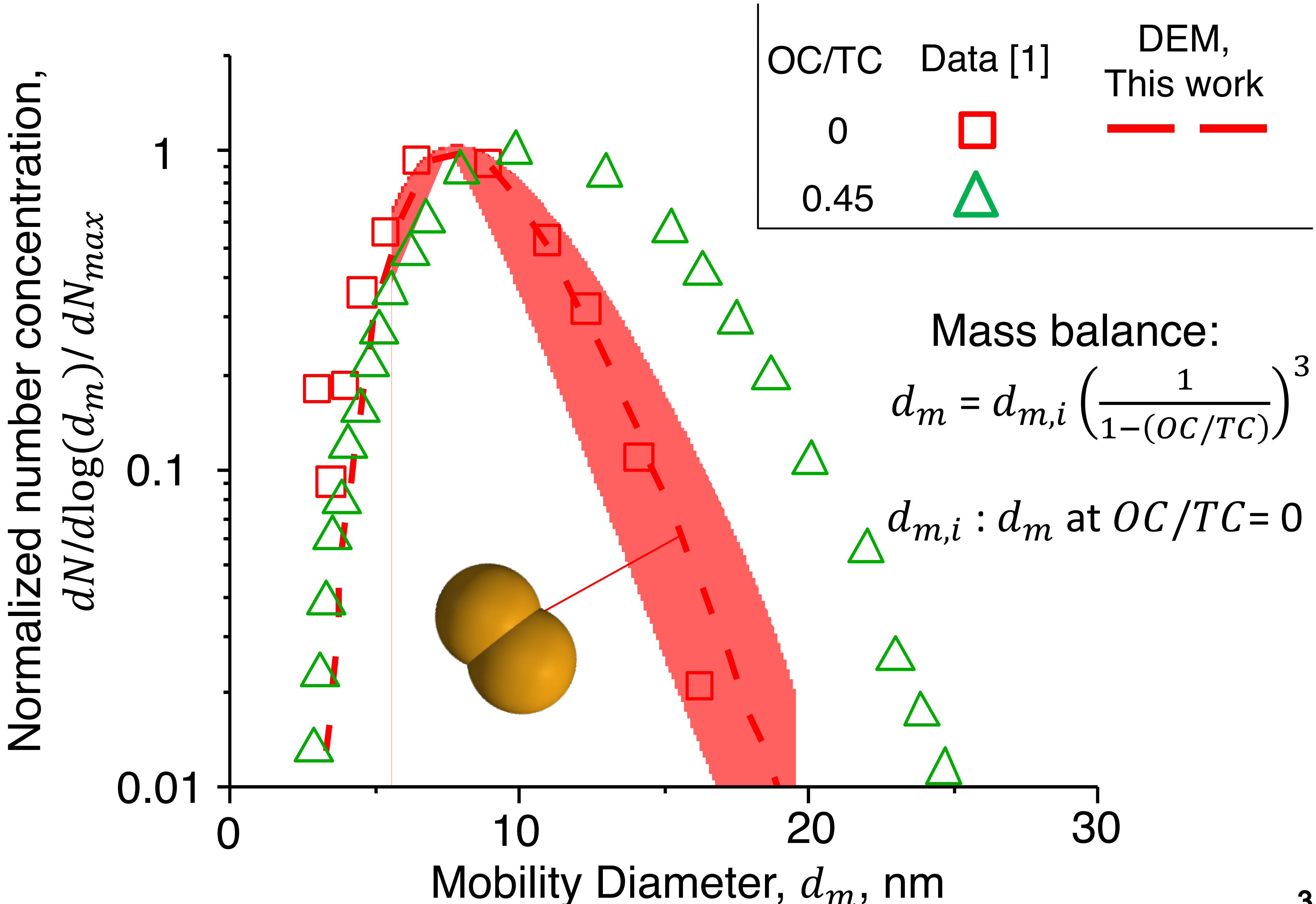


[1] Maricq, M.M., *Aerosol Sci. Technol.* **48** (2014) 620.

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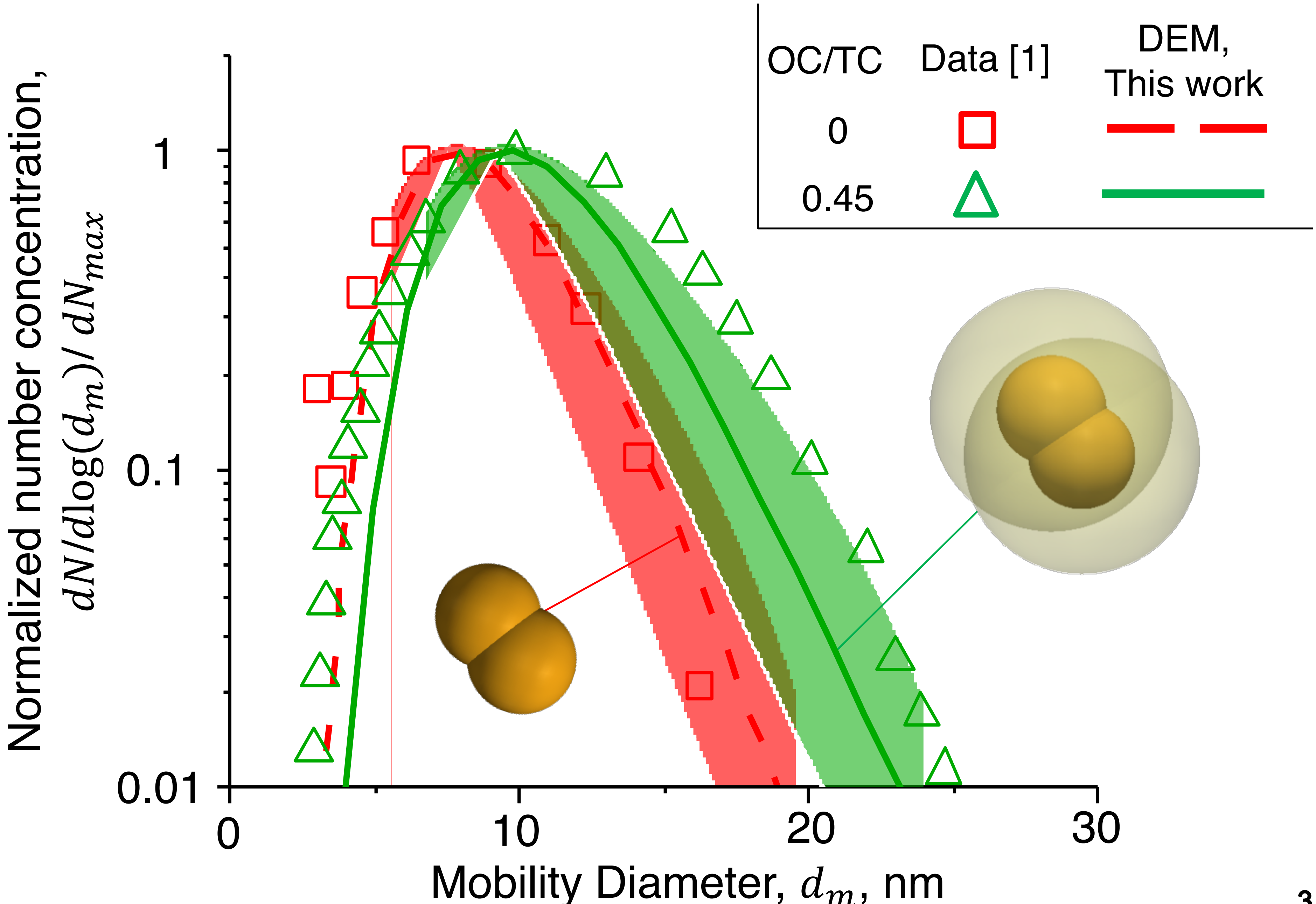




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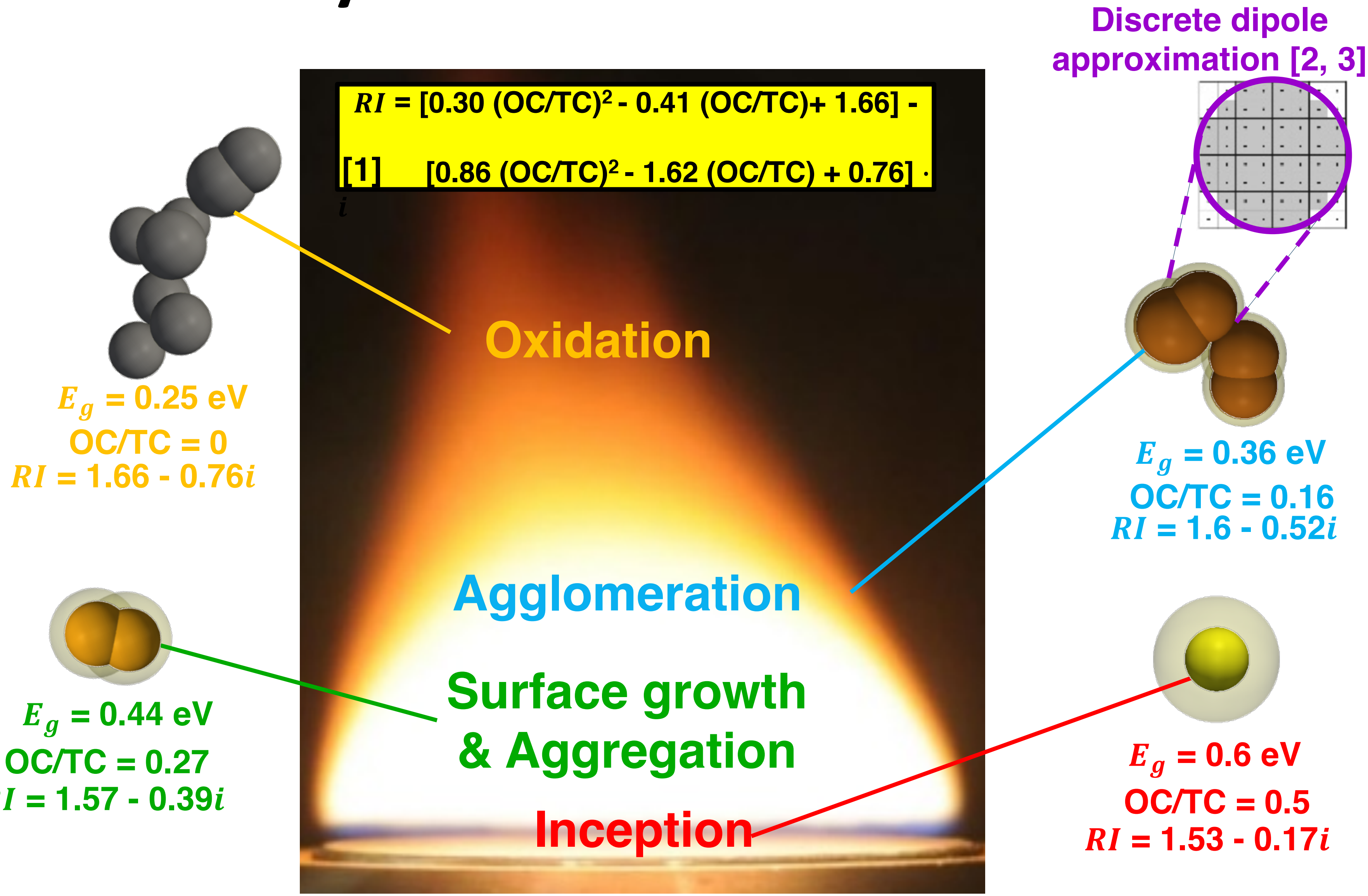
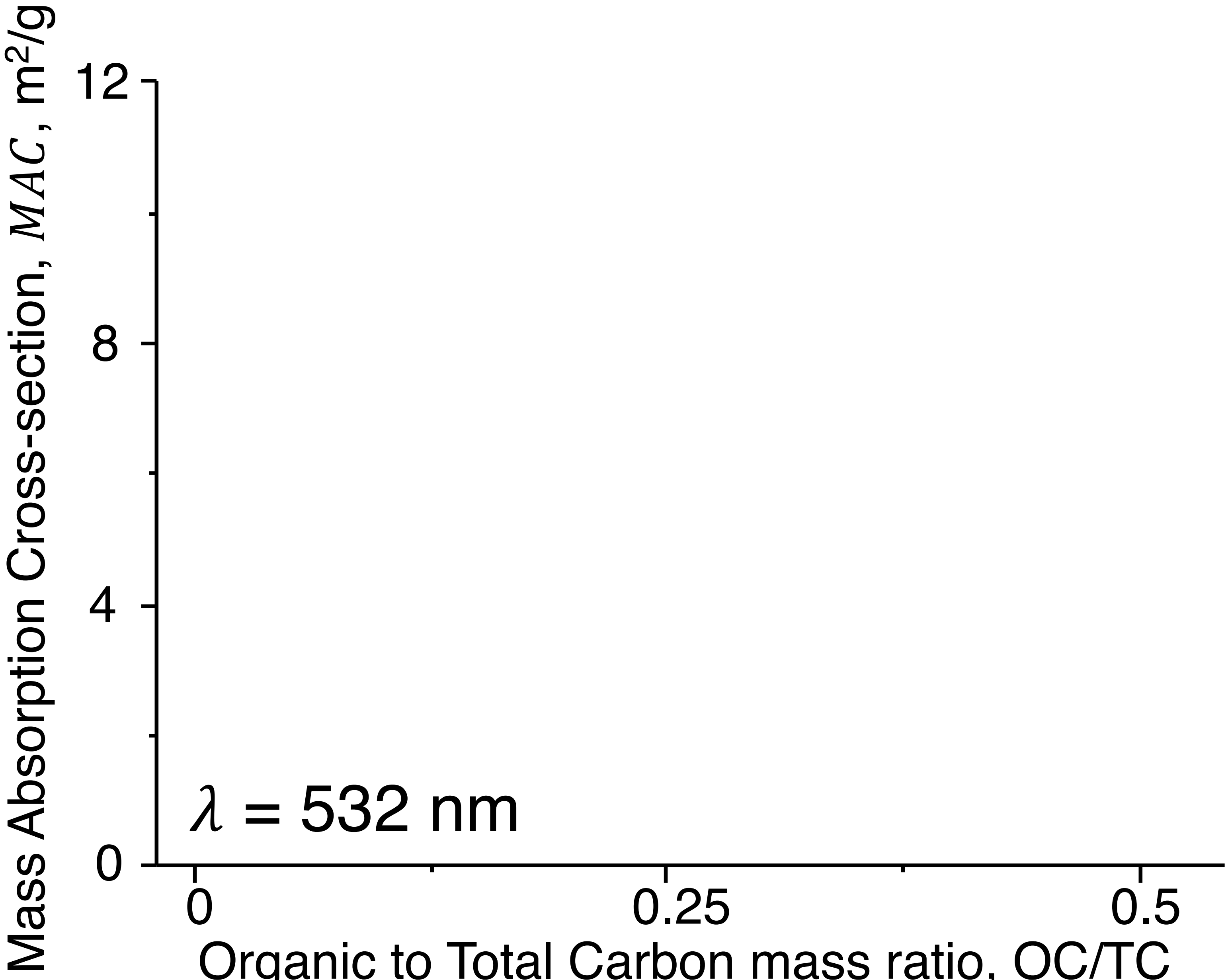




[1] G.A. Kelesidis, C.A. Bruun, S.E. Pratsinis, Carbon 172 (2021) 742-749.
[2] G.A. Kelesidis, M.R. Kholghy, J. Zurcher, J. Robertz, M. Allemann, A. Duric, S.E. Pratsinis, *Powder Technol.* **365** (2020) 52.
[3] G.A. Kelesidis, S.E. Pratsinis, *Proc. Combust. Inst.* **37** (2019) 1177.

# Impact of OC on *MAC* dynamics



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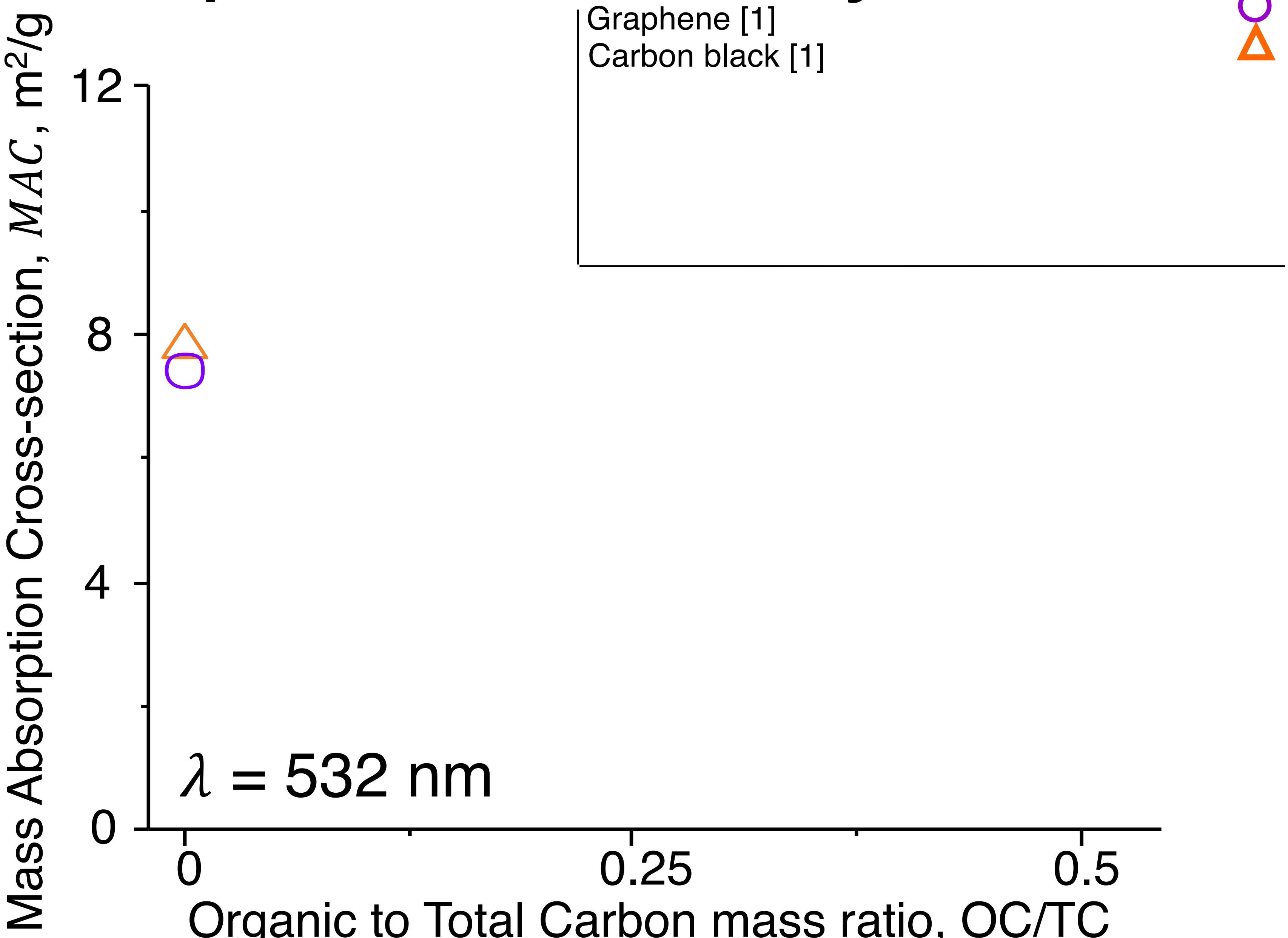



[1] C.D. Zangmeister, R. You, E.M. Lunny, A.E. Jacobson, M. Okumura, M.R. Zachariah, J.G. Radney, Carbon 136 (2018) 85-93.

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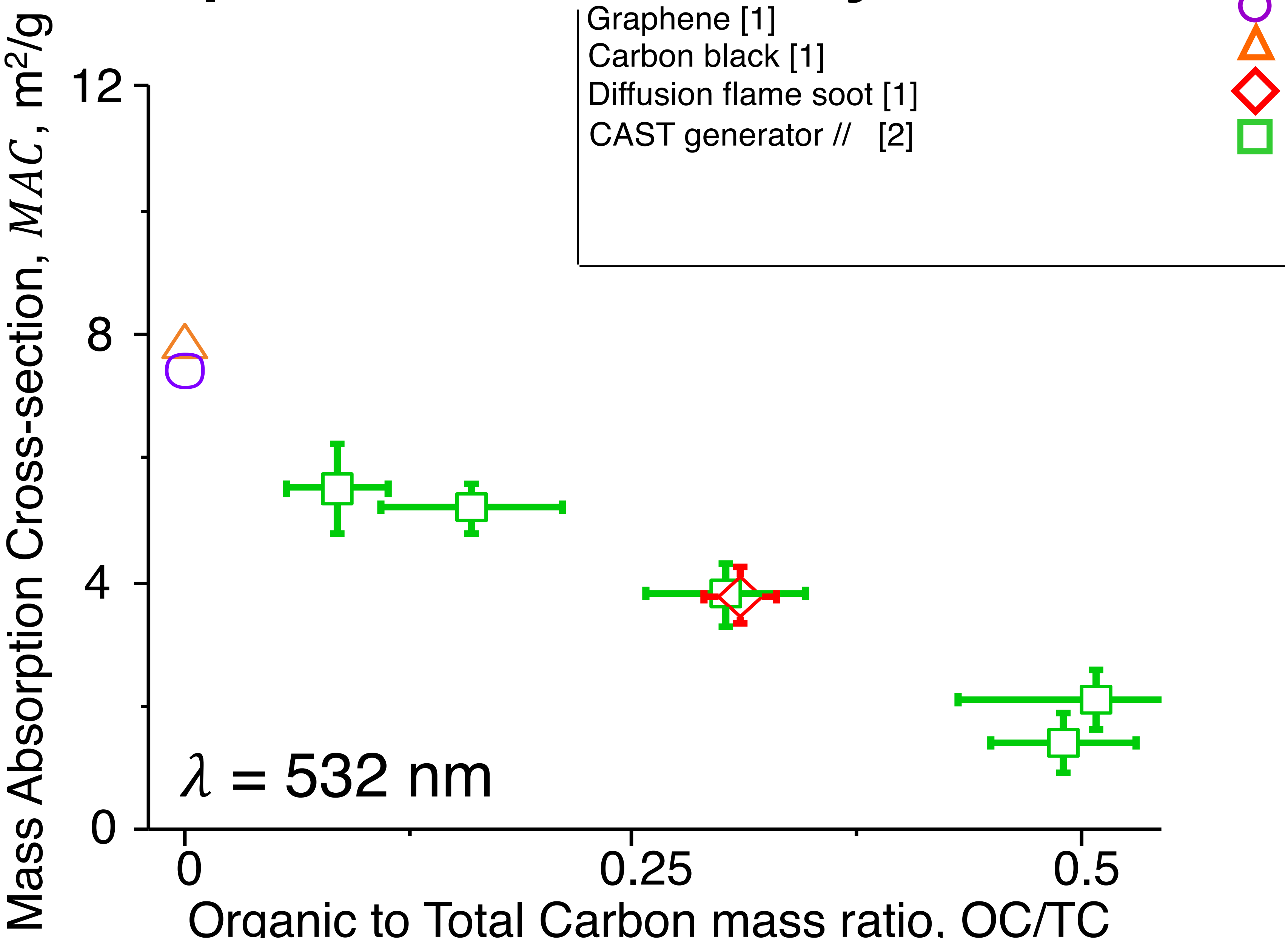



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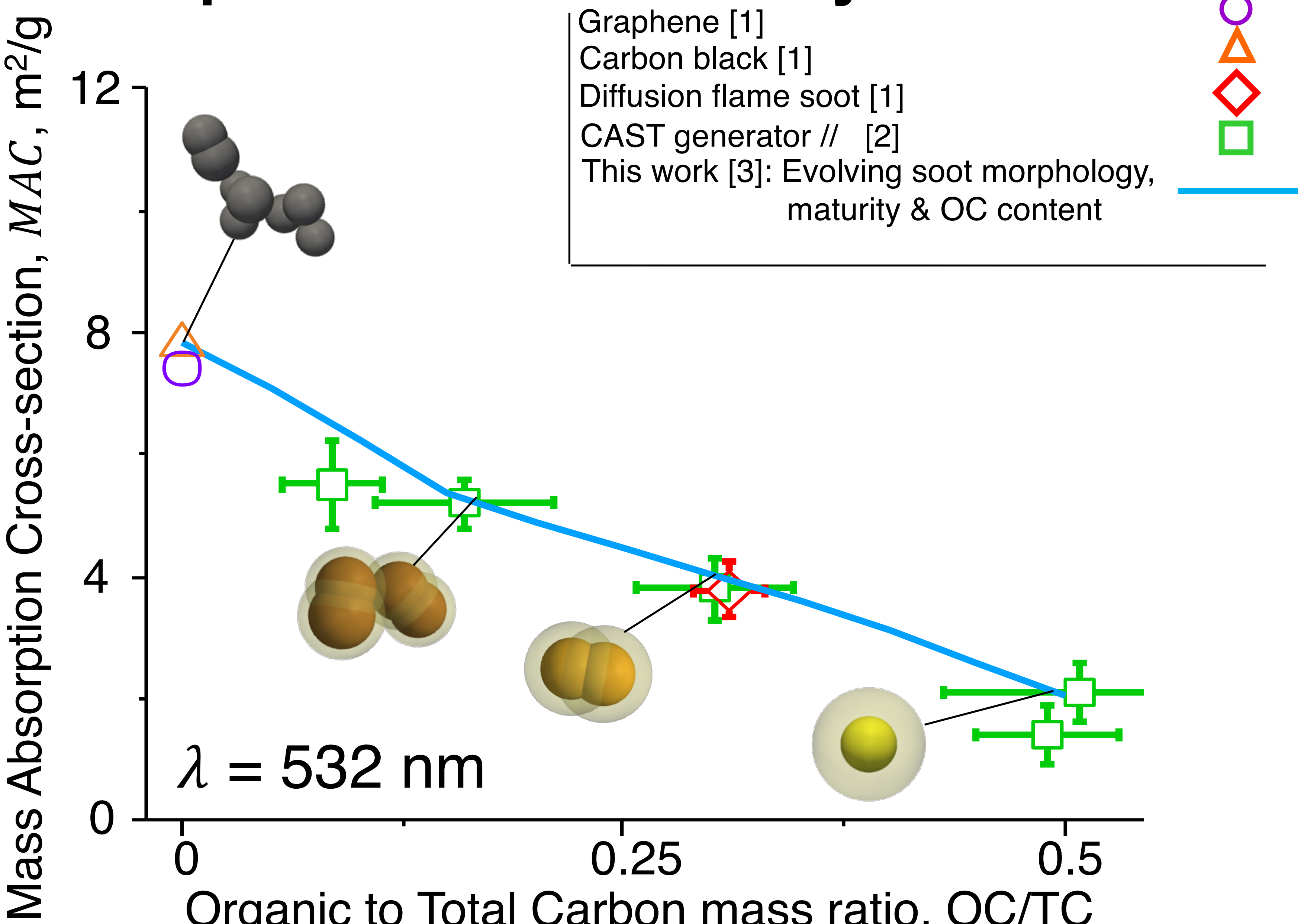


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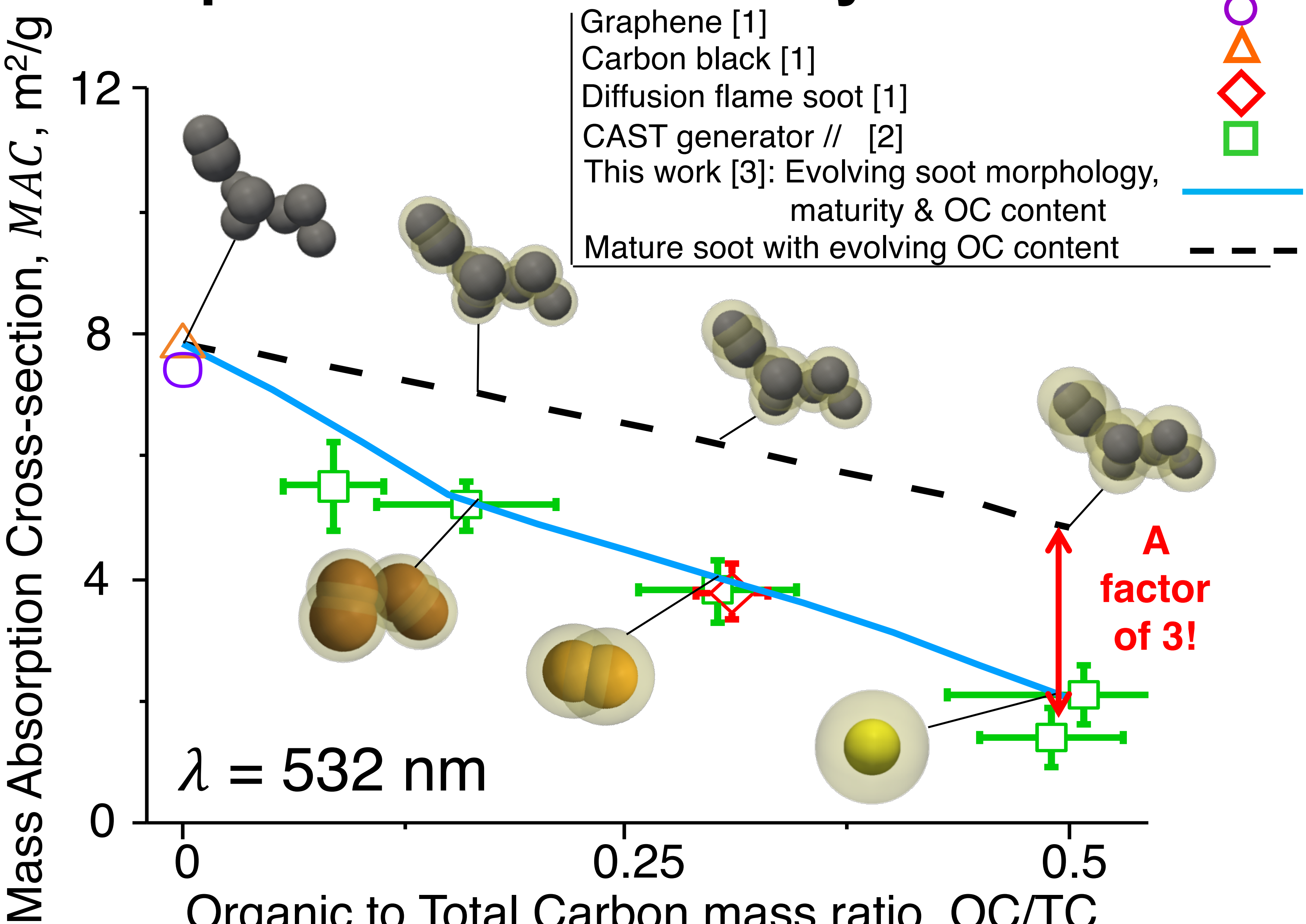



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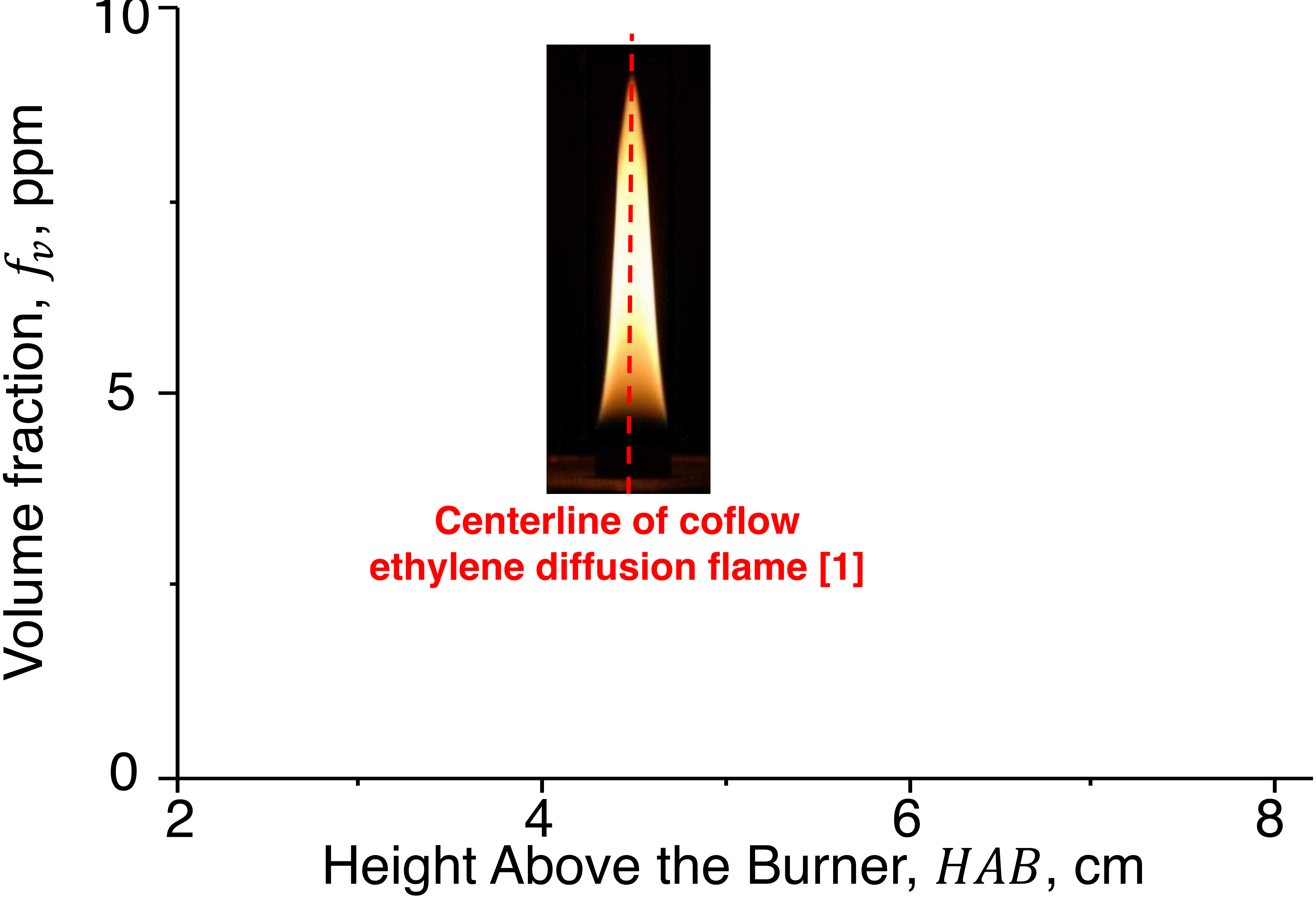
[3] G.A. Kelesidis, C.A. Bruun, S.E. Pratsinis, Carbon 172 (2021) 742-749.

# Soot $f_v$ dynamics in the Santoro flame




[1] R. Puri, T.F. Richardson, R.J. Santoro, R.A. Dobbins, *Combust. Flame* **92** (1993) 320.

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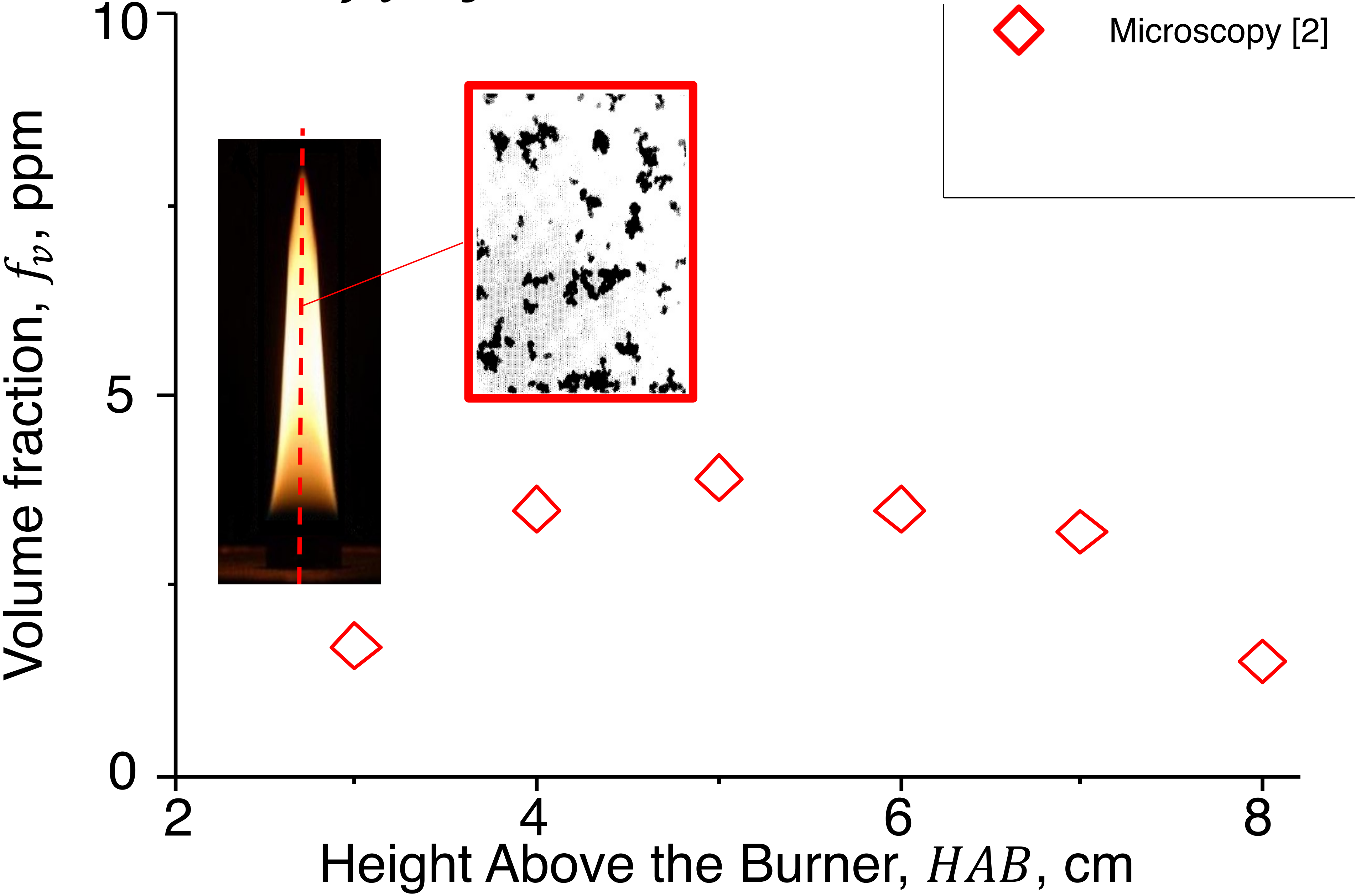



[1] R. Puri, T.F. Richardson, R.J. Santoro, R.A. Dobbins, *Combust. Flame* **92** (1993) 320.
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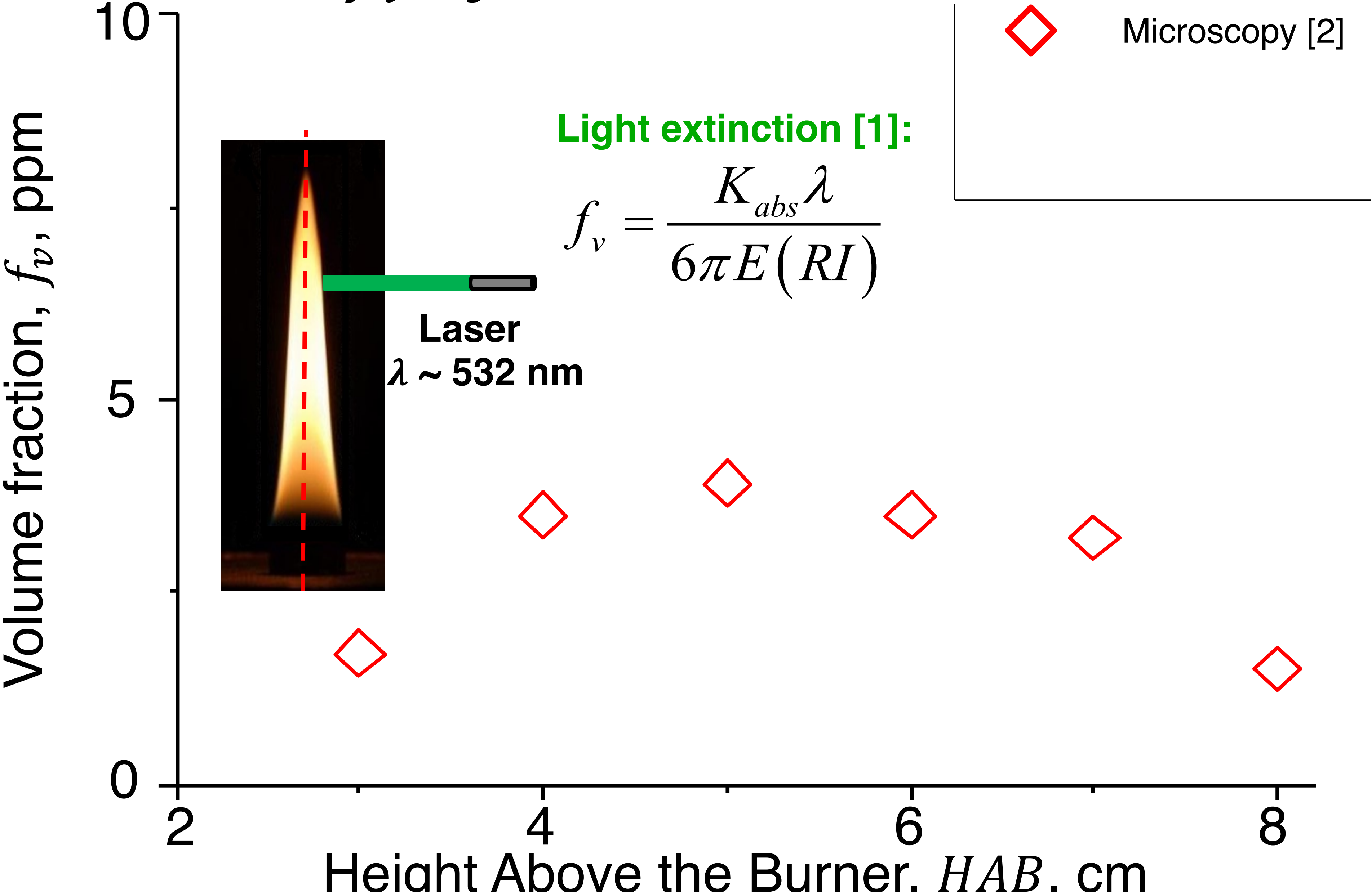


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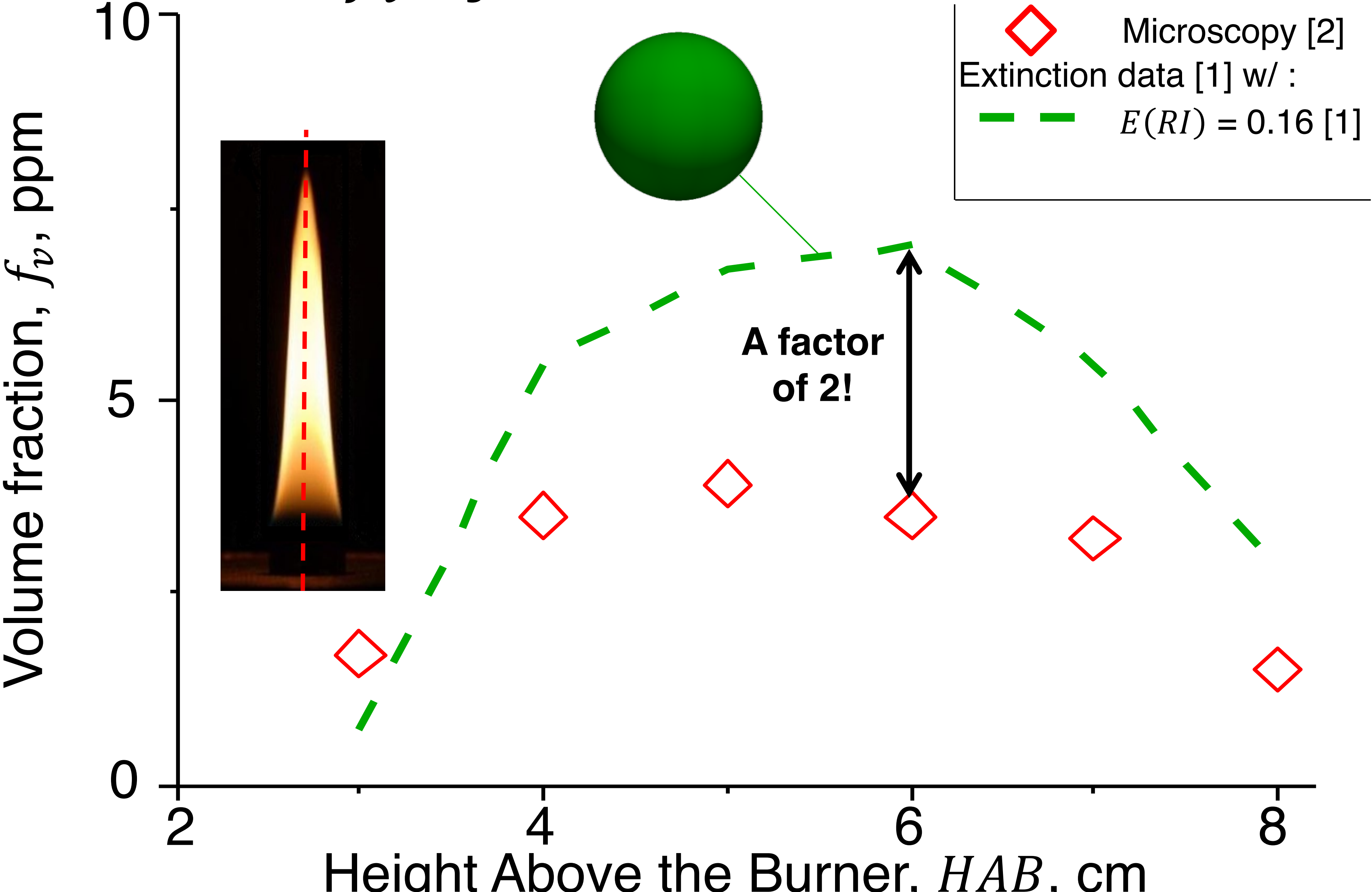



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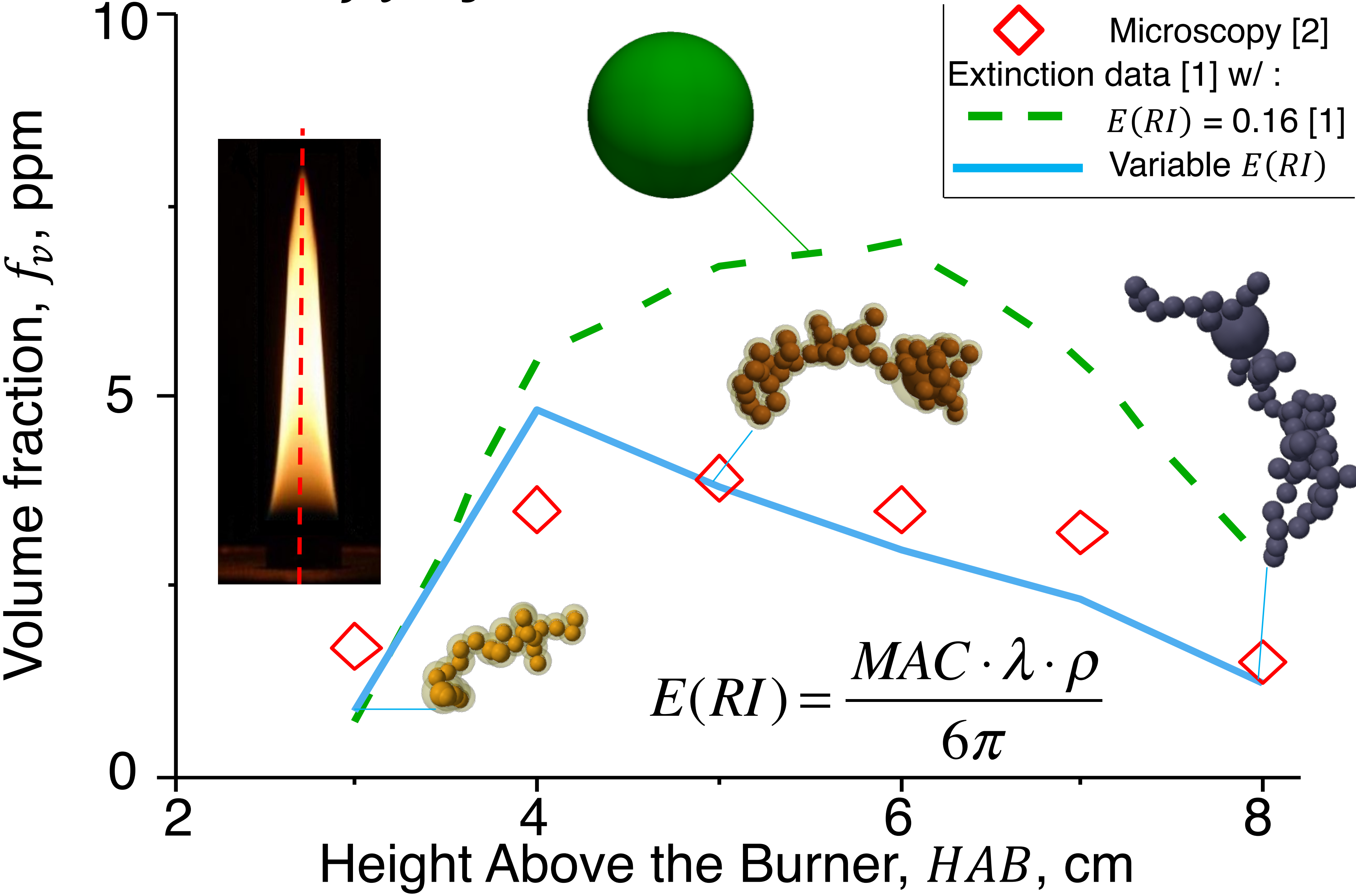



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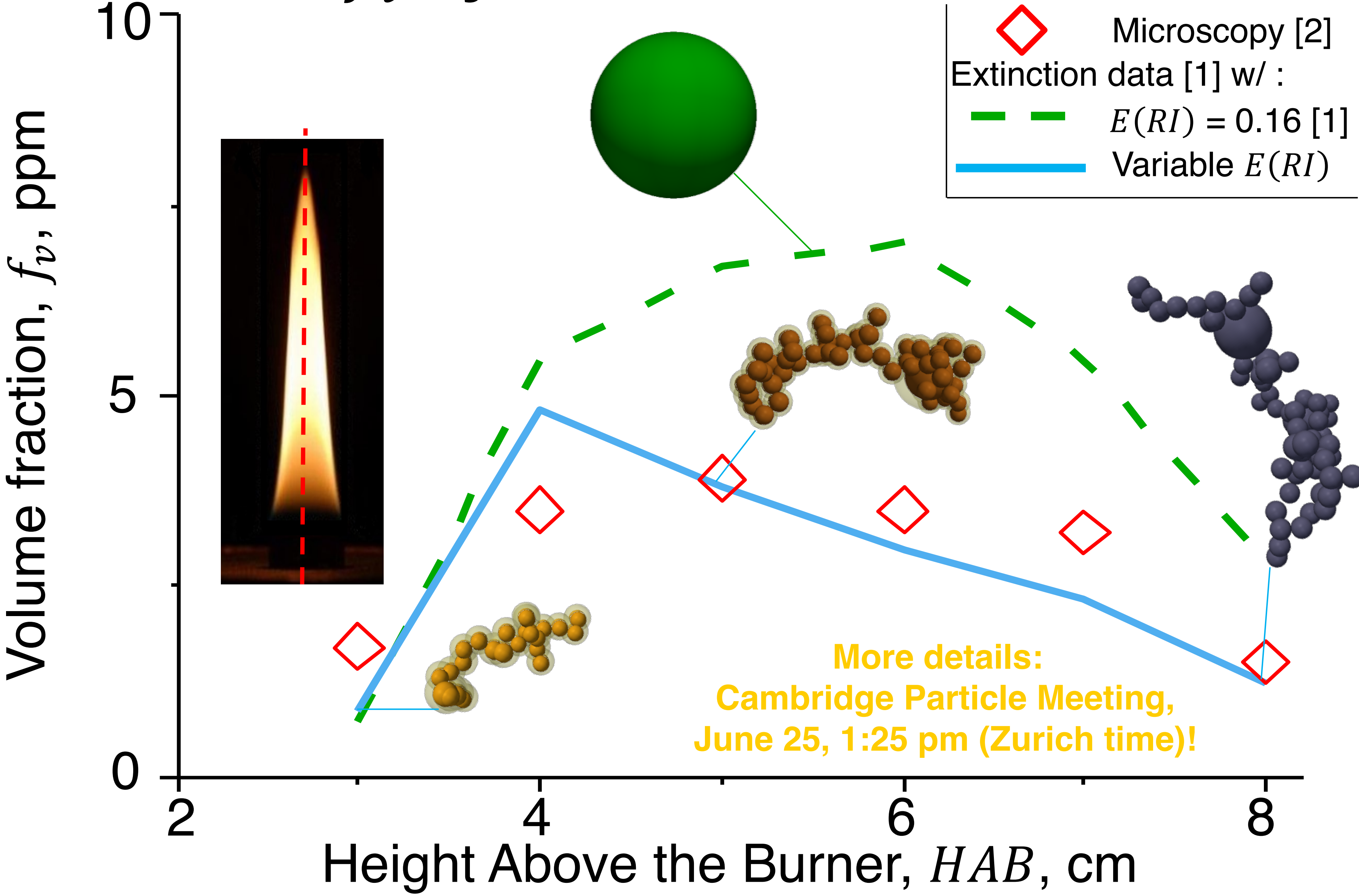



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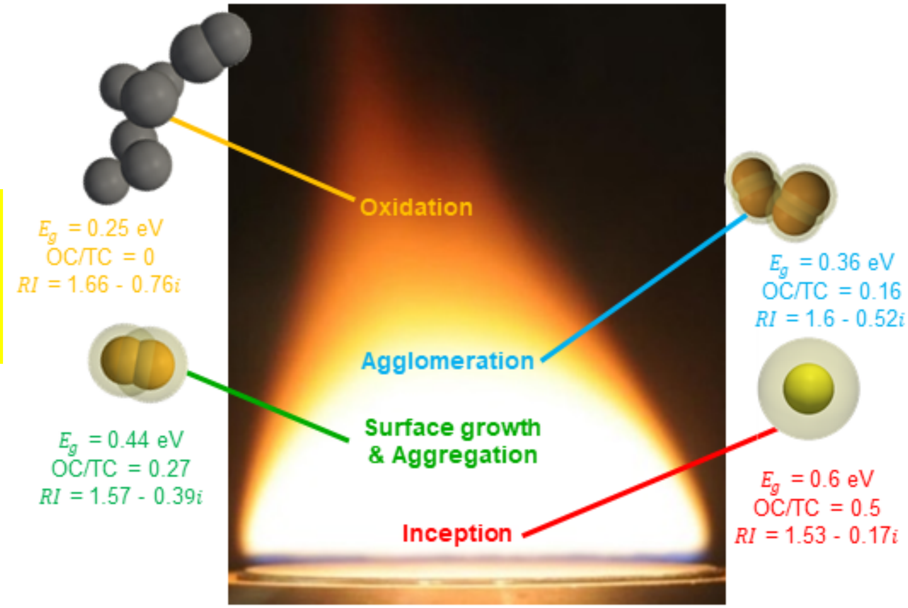
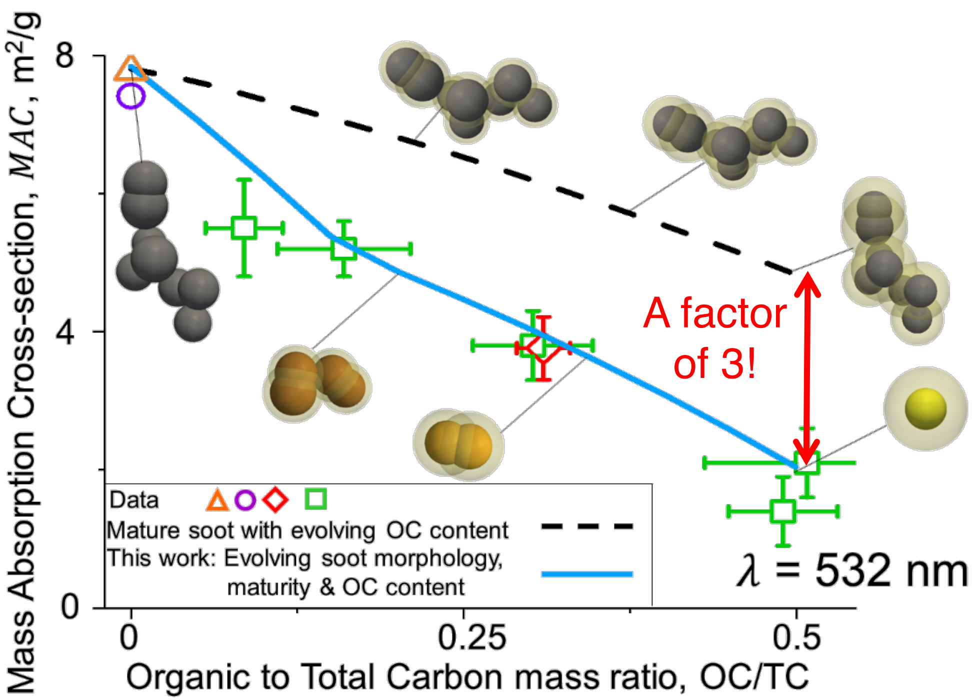
# Conclusions

- New relation for soot refractive index, *RI*, accounting for soot morphology, maturity & organic carbon (OC) content:

$$RI = [0.30\,(OC/TC)^2 - 0.41\,(OC/TC) + 1.66] - [0.86\,(OC/TC)^2 - 1.62\,(OC/TC) + 0.76] \cdot i$$




- Neglecting the evolving soot maturity & morphology as a function of OC content overestimates soot *MAC* up to **a factor of 3**!

- The soot *RI & MAC* derived here from first principles can be used for accurate laser diagnostics of soot $f_v$!



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