

Supplementary Information for Room temperature dynamics of atomic clusters adsorbed on graphene: a machine-learning force field molecular dynamics study

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^c Imec, Kapeldreef 75, B-3001 Leuven, Belgium

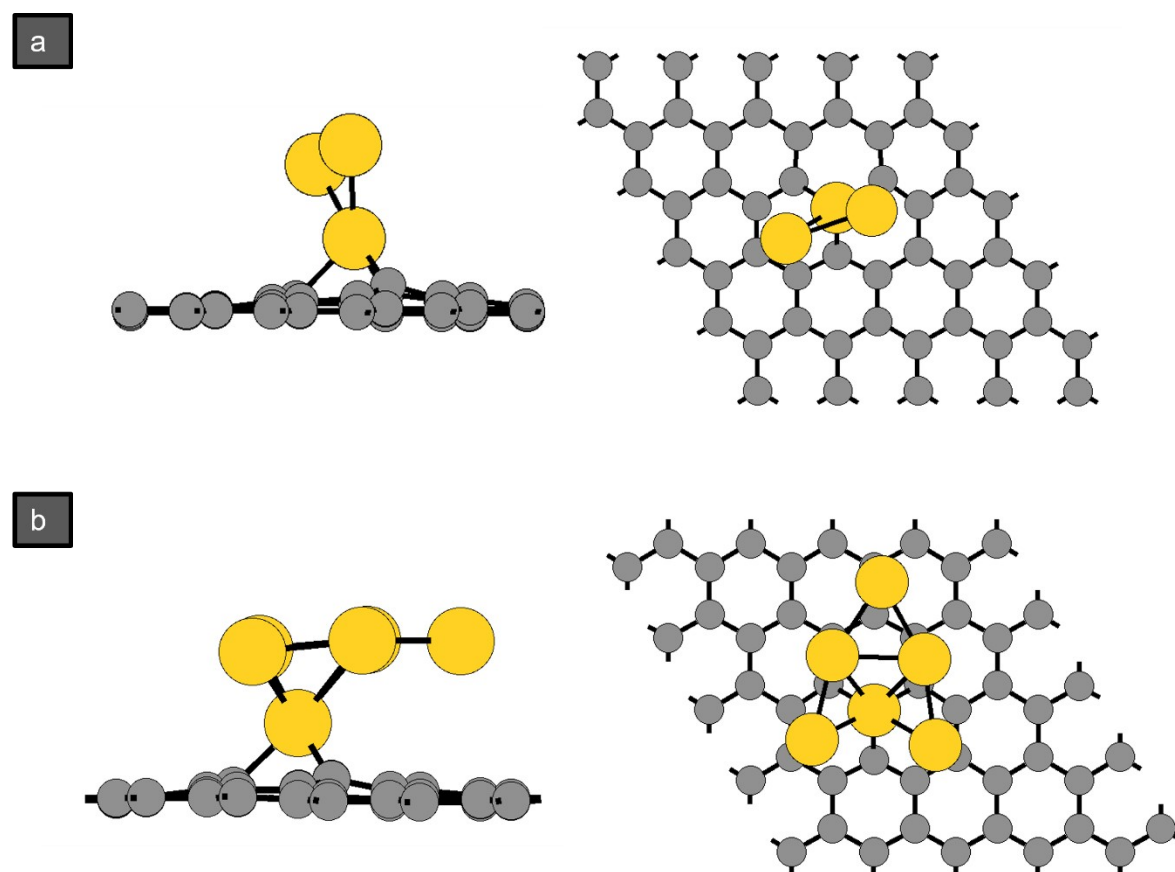


Figure S1: The relaxed geometrical configurations for Au₃ (a) and Au₆ (b) clusters adsorbed on graphene with a single carbon vacancy.

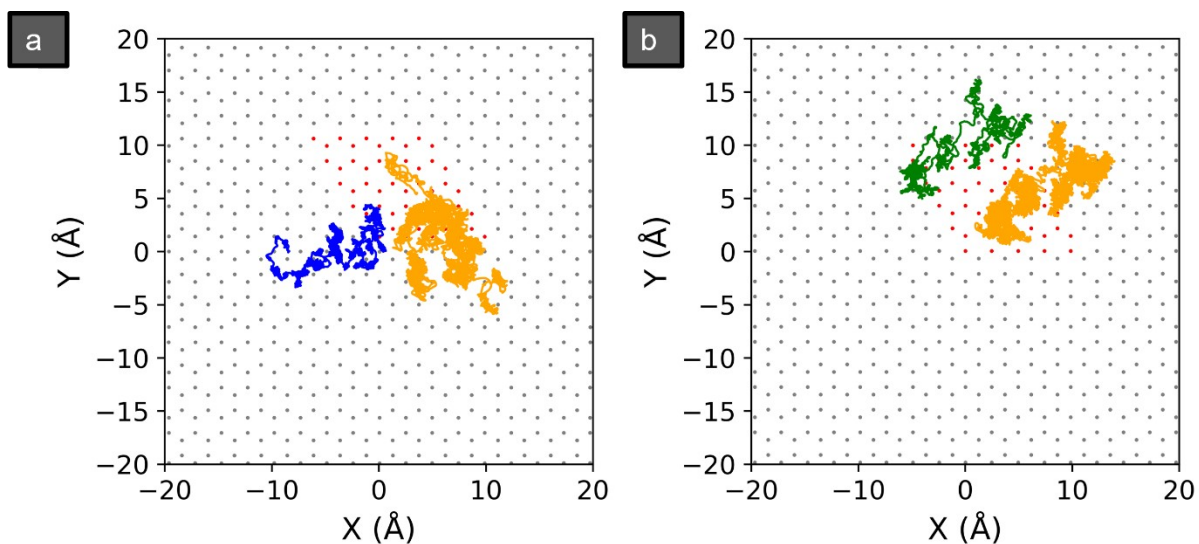


Figure S2: The trajectories of Au_3 (a) and Au_6 (b) cluster's center of mass during the MD simulations on graphene surfaces with MMA residues. The blue (green) line corresponds to the center of mass of the Au_3 (Au_6) cluster, the orange corresponds to the center of mass of MMA residue.

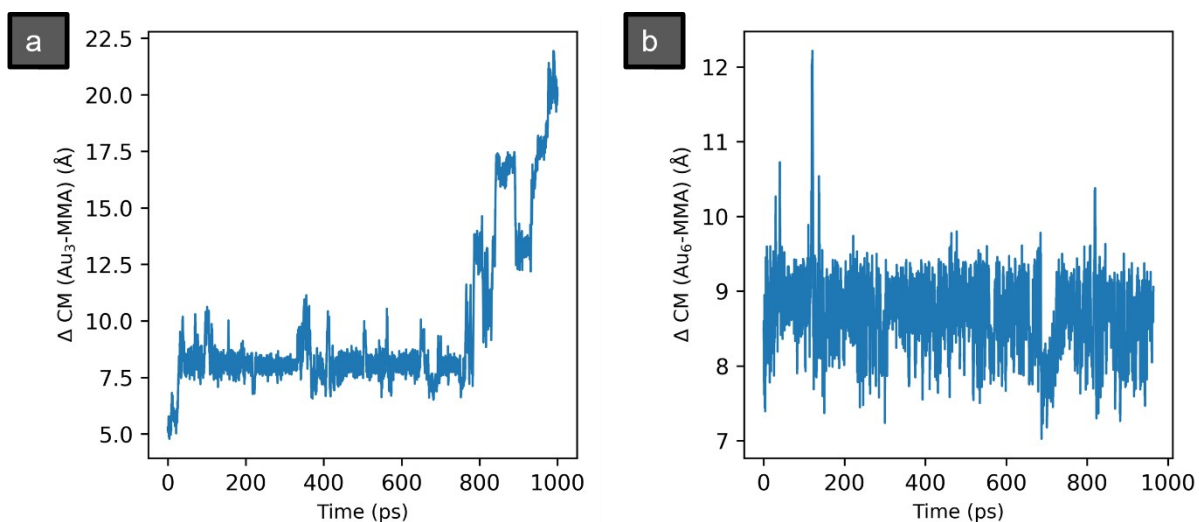


Figure S3: The difference between the center of mass of cluster ((a) Au_3 & (b) Au_6) and MMA residue for the entire MD simulation run of 1ns.

Simulation on 10x5 graphene supercell with MMA residue

To address the reliability of the conclusion that the presence of MMA residues reduces the diffusion of the Au_n cluster, we performed a simulation on 10x5 graphene supercell adsorbed with one Au_3 cluster and one MMA molecule (structure shown in Fig. S4).

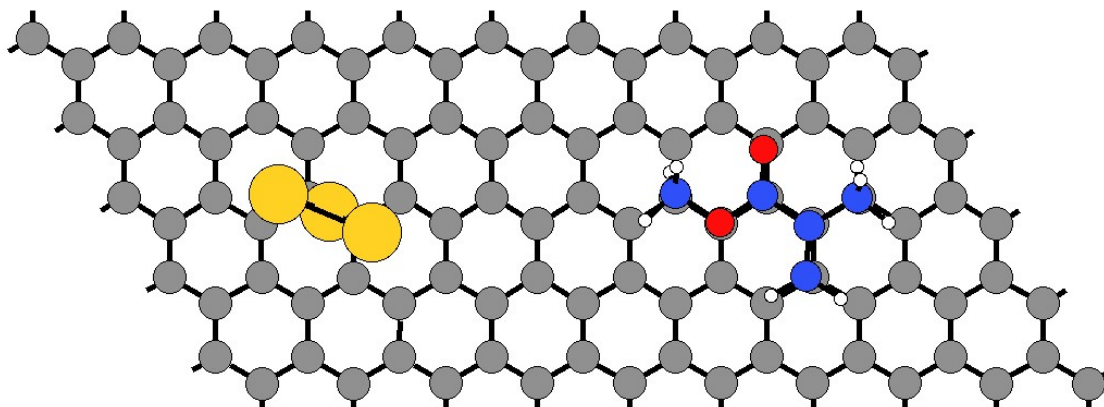


Figure S4: Relaxed geometrical configurations of Au_3 and MMA residue ($C_5H_8O_2$) adsorbed on a 10x5 graphene supercell .

The MD simulation was performed for 1 ns with a timestep of 0.5 fs. From the trajectory of the cluster's center of mass, the diffusion area was found to be 2.68 nm^2 , which is of the same order of magnitude but higher than the value obtained from the 5x5 supercell (0.86 nm^2). The difference can be attributed to the reduced density of MMA in the larger supercell. When compared to the diffusion area of a Au_3 cluster adsorbed on pristine graphene (9.9 nm^2) the diffusion area is still greatly suppressed. This additional simulation confirms our claim that the presence of MMA residues significantly limits the movement of Au_n clusters. Furthermore, we analyzed the MSD of the cluster's center of mass and computed the slope from the log-log plot of MSD vs τ (Fig. R2). The slope value at τ_{cut} was found to be 0.705 (with the most probable value being 0.8 as shown in the inset of Fig. R2), which is in line with value computed for the simulation with 5x5 a supercell. This supports the claim of sub-diffusive behavior for Au_n clusters on graphene with MMA residues.

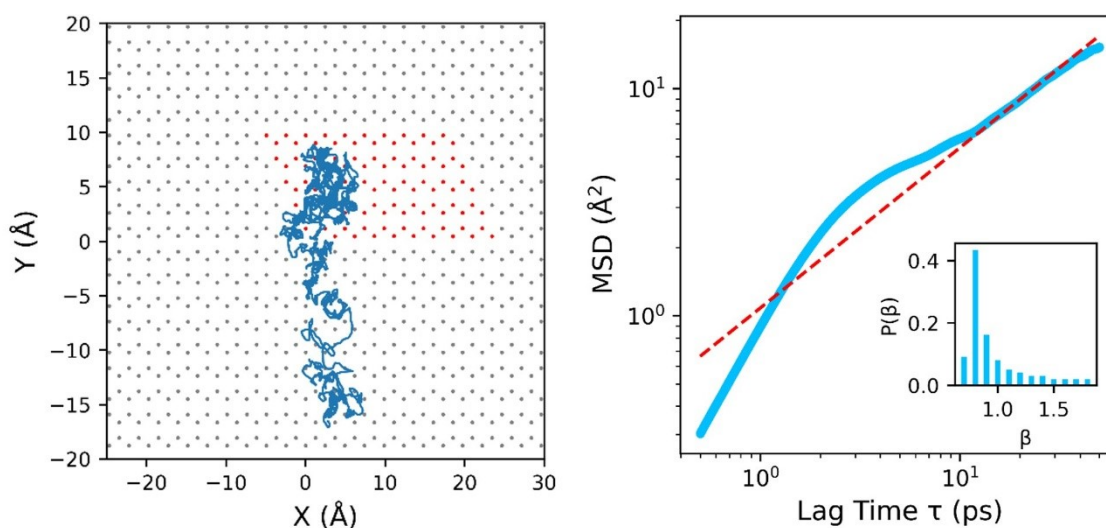


Figure S5: The trajectories of Au₃ cluster's center of mass during the MD simulations on graphene surfaces with MMA residues (right). Log-log plot of MSD vs lag time, with the red dashed line representing the power law fit obtained at $\tau_{\text{max}}=50$ ps for Au₃ clusters absorbed on graphene layers with MMA residues (left). Inset: The probability distribution histogram of the extracted slope β for multiple time interval $[0:\tau]$ as computed from trajectories

Benchmarking PBE-D3(BJ)

We compared the DFT-D3 approach with a domain-based pair natural orbital coupled-cluster approach DLPNO-CCSD(T), using coronene (C₂₄H₁₂) as a molecular model of graphene using the ORCA package¹. We computed the interaction energy curve of Au₂ cluster (smallest possible cluster size) as a function of Au₂-coronene separation using def2-TZVPD basis set²⁻⁷. The obtained results are shown in Figure S6.

Both DLPNO-CCSD(T) and PBE-D3(BJ) predict the same equilibrium bond distance, $Z \approx 2.31$ Å. DLPNO-CCSD(T) yields a deeper minimum (−1.19 eV), consistent with its more complete treatment of electron correlation and dispersion. The PBE-D3(BJ) methods yields a 0.33 eV lower interaction energy of -0.85 eV, but it reproduces the shape of the curve. Pure PBE strongly underestimates the interaction energy and provides a too short Au₂ – C₂₄H₁₂ distance.

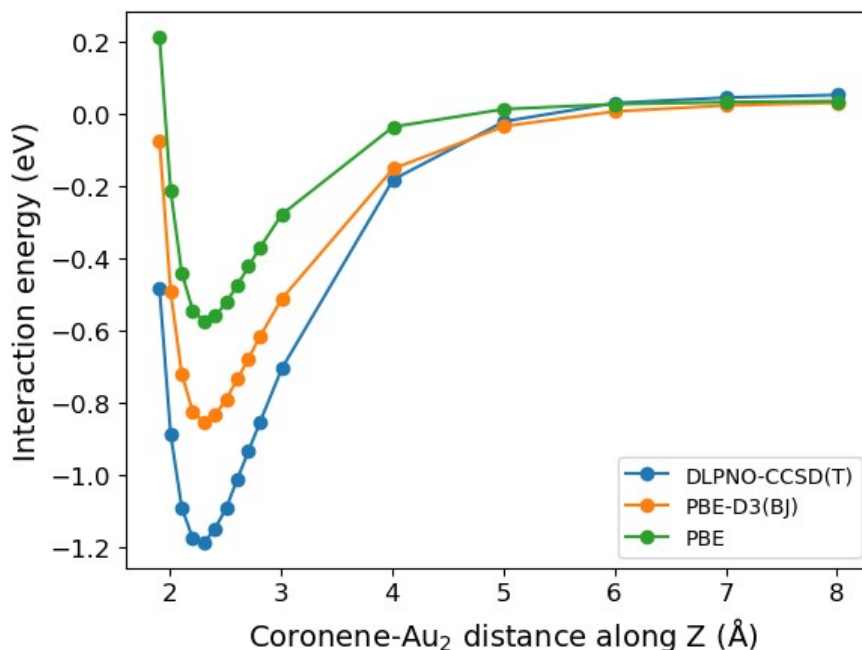


Figure S6: Interaction energy between Au₂ cluster and coronene (C₂₄H₁₂) using different methods

Because diffusion depends on the lateral corrugation of the potential energy surface, we additionally evaluated three adsorption sites (top, bridge, hollow). The interaction energy and deviations from DLPNO-CCSD(T) are summarized in Table S1. Across all sites PBE-D3(BJ) systematically underestimated the interaction energy by ~ 0.33 eV but preserves the relative energy differences between the adsorption sites, which is essential for the diffusion barriers and cluster mobility.

Position	Binding Energy (eV)		ΔE (eV)
	PBE-D3(BJ)	CCSD(T)	
Top	-0.8532	-1.1870	0.33
Bridge	-0.8212	-1.1565	0.34
Hollow	-0.4998	-0.8310	0.33

Table S1: Binding energy evaluated at three different adsorption sites

These results demonstrate that PBE-D3(BJ) captures the interaction profile (correct equilibrium distance and similar curvature) despite an underestimation of the adsorption energy relative to DLPNO-CCSD(T). For the purposes of this study (cluster diffusion and structural trends on graphene) PBE-D3(BJ) provides an acceptable compromise between accuracy and computational feasibility.

VASP POSCAR File for Au₃ cluster on Pristine Graphene

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VASP POSCAR File for Au₆ cluster on Pristine Graphene

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VASP POSCAR File for Au₃ cluster on Single Carbon Vacancy Graphene

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VASP POSCAR File for Au₆ cluster on Single Carbon Vacancy Graphene

Defect-Graphene-Au₆

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0.8657314686656932 0.5238124692932118 0.4870607923499364
0.8659483732259048 0.7244240957502015 0.4872608607966313
0.8654649873285933 0.9244629522218801 0.4869618245863307
0.4407185348250025 0.6759364287149339 0.6737591963896747
0.2726680648849182 0.4397621872912865 0.6633180214309178
0.6625058273810467 0.8813672070015386 0.6725965685140309
0.4651647369819116 0.5230845832833992 0.5764749090396819
0.6575938763574669 0.6648650787457484 0.6732913037610331
0.5650454974049239 0.4245498299607249 0.6602194850442018

VASP POSCAR File for Au₃ cluster Graphene with MMA residue

Graphene-MMA-Au3

1.0000000000000000
12.3000000000000007 0.0000000000000000 0.0000000000000000
-6.1499999999999977 10.6521124665485960 0.0000000000000000
0.0000000000000000 0.0000000000000000 25.6960000000000015

C O H Au

55 2 8 3

Direct

0.0034232204885427 0.9975222767279135 0.3658020656071912
0.0713952448662667 0.1320244097945462 0.3697673618500232
0.0036747529515679 0.1997203233353559 0.3704027761407076
0.0712999409788111 0.3336779158383720 0.3667847663415031
0.0042143561027714 0.3995275609485702 0.3653330401916222
0.0709231739225729 0.5327878844135938 0.3638394388166830
0.0041354593732876 0.5992435194166106 0.3631941546882942
0.0707948559403988 0.7324637270542098 0.3630252392400664
0.0039748027473365 0.7988343838430509 0.3630502787227954
0.0707504597788997 0.9320181195746855 0.3639689204704553
0.2042251486568674 0.9991707616984087 0.3636135874776016
0.2713217280359856 0.1326596805660998 0.3632057036116052
0.2057873754685460 0.1999461456509906 0.3649723370561659
0.2712677835059480 0.3328662129997753 0.3628931641784163
0.2042623518191817 0.3995587265933906 0.3638861965997435
0.2709043448689386 0.5327238549494169 0.3622663967055288
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0.2708379540341355 0.7327080672531636 0.3625537779714065
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0.4709240838857482 0.1326383030608724 0.3621511314894477
0.4045008164282322 0.1994305623106385 0.3618430432545665

0.4709295120866699 0.3326738380033589 0.3608024805906069
0.4043632723471475 0.3993986219524288 0.3606158829761341
0.470868852653964 0.5326742081666396 0.3598766226249239
0.4041954725301551 0.5993047742020181 0.3605531859869231
0.4707548064104685 0.7325965545647648 0.3607647829218834
0.4041457912385908 0.7992961197221007 0.3618527925771460
0.4707268248097520 0.9326202782206892 0.3623670255257281
0.6040727730016755 0.9992347191154707 0.3629204297135402
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0.6708056968720442 0.3325979587336718 0.3618927745515066
0.6042479920572035 0.3992786288951820 0.3606992502382766
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0.8038812369871025 0.1991576482383408 0.3652339061267895
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0.8041859767930504 0.3991827188504402 0.3630367499785265
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0.8707159207941189 0.7323905457146651 0.3623647467228892
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0.6767621484352375 0.4045029547526511 0.4953617932033509
0.4653175804332861 0.5379382680351057 0.4943645892382520
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0.5838551689360827 0.5326252711895165 0.4944728520421364

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0.7448611053377121 0.4652935672183816 0.4660204394423744
0.7200816676493389 0.4325634739027606 0.5340254064498424
0.6461572277589553 0.3057059662632398 0.4878981191190590
0.5481222668925412 0.7283244456897933 0.4666769433918390
0.5247918414685557 0.7125454674931717 0.5342928123060844
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0.2661482913117013 0.4373333596365825 0.4924278454373265
0.3426397945776074 0.3398111205176804 0.4914029453297246
0.0557951626538298 0.1510241498780758 0.4564963237647461
0.1565626951154044 0.0653292417540072 0.5251795838966657
0.0408318417936044 0.1961630797921643 0.5541690581814436

VASP POSCAR File for Au₆ cluster Graphene with MMA residue

Graphene-MMA-Au6

1.0000000000000000

12.3000000000000007 0.0000000000000000 0.0000000000000000

-6.1499999999999977 10.6521124665485960 0.0000000000000000

0.0000000000000000 0.0000000000000000 25.6960000000000015

C O H Au

55 2 8 6

Direct

0.0037023080661740 0.0038470397772201 0.3640897872515723

0.0703721037678946 0.1371822871248796 0.3641948864262972

0.0037234333462450 0.2038661634706997 0.3641312419385159

0.0704006435411060 0.3372277935102872 0.3632539436176145

0.0037359534378680 0.4039702855267464 0.3622505858149836

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0.0036833402533460 0.8037961601899184 0.3623234011110839

0.0704003181768869 0.9371731954727025 0.3630607138628505

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0.2704147746464400 0.1372147869170064 0.3626049674024401

0.2037391970323625 0.2038655010527037 0.3634608612114647

0.2704212734143496 0.3372266695262098 0.3628967879557976

0.2037809462093492 0.4039590488599814 0.3627169161890365

0.2703617390887842 0.5372820749088376 0.3614354803438644

0.2037153049546845 0.6039525271676638 0.3604938429450684

0.2703474136403017 0.7372362398948766 0.3600344101675432

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References

1. Neese, F. Wiley Interdiscip. Rev.: Comput. Mol. Sci., 2022, 12, 1, e1606
2. D. Andrae, U. Haeussermann, M. Dolg, H. Stoll, H. Preuss, Theor. Chim. Acta, 1990, 77, 123-141.
3. F. Weigend and R. Ahlrichs, Phys. Chem. Chem. Phys., 2005, 7, 3297.
4. D. Rappoport and F. Furche, J. Chem. Phys., 2010, 133, 134105.
5. F. Weigend, Phys. Chem. Chem. Phys., 2006, 8, 1057.
6. A. Hellweg, C. Hattig, S. Hofener and W. Klopper, Theor. Chem. Acc., 2007, 117, 587.
7. A. Hellweg and D. Rappoport; Phys. Chem. Chem. Phys., 2015, 17, 1010.