THESES OF DOCTORAL (Ph.D.) DISSERTATION

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Automating the development of high-dimensional potential energy surfaces with robust electronic structure methods

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I. Introduction and research goals

Both computational and experimental methods of studying elementary gas-phase reactions belong to two broad approaches: macroscopic and microscopic.

In the macroscopic approach, the usual thermodynamic and kinetic parameters of enthalpy, entropy and rate constants are either measured experimentally or computed at the transition state of the reaction with quantum chemical methods and the familiar Eyring equation. While this is often a practical approach, the results tell very little about the microscopic details of a reaction, such as the steric effects evident in angle-dependent reaction probabilities, the vibrational and rotational excitation distributions of products or the effects of mode-specific vibrational excitation of reactants on reactivity. Accessing the microscopic quantities is much more difficult however.

Experimentally, one may have no other option than building an elaborate vacuum apparatus to measure the scattering angle and velocity distributions of products formed in the crossing point of two carefully prepared beams of ions or molecules, while theory is confronted with having to solve immensely difficult reactive scattering problems. The microscopic quantities are worth obtaining nevertheless, as it is one of the few ways of learning more about the dynamics of a reaction. Especially interesting are the results obtained from reactant states where a particular (ro)vibrational mode is excited, as some reactions may be selectively promoted using a tunable laser. Furthermore, as all macroscopic kinetics stem from the microscopic behaviour of the system it is in principle possible to accurately predict reaction rates even if the assumptions of transition state theory are not met. Achieving that in practice hinges on one's ability to simulate the reactive scattering of molecules.

One of the great hurdles is computing accurate potential energy values at a huge number of molecular geometries to integrate the equations of motion, as the computational cost of this is intractable even with the latest computers and theoretical methods. This can be circumvented by creating an efficient surrogate model based on a moderate number of accurate potential energy values, and using the surrogate model to run the scattering simulations instead. A surrogate modelling method that has been successful in the last 20 years is the fitting of analytical potential energy (hyper)surfaces (PESs) using permutationally invariant polynomials (PIPs). Today, the difficulties of constructing fitting sets remain the primary inhibitors of reaction dynamics simulations, and developing reliable methods for doing so would open the way for a much more widespread use of the microscopic approach of studying reactions.

The quality of the dataset used for PES fitting is critically important, as is how the sparse sampling of the vast $3N - 6$ (where N is the number of atoms) dimensional space spanned by the molecular degrees of freedom is achieved. Finding the most practical methods of sampling the configuration space with a bias towards chemically

important regions is an open research problem. Given that the potential energies of the molecular geometries in a fitting set are computed with a quantum chemistry method that solves the electrons' Schrödinger equation only approximately, another open question is how these approximations affect the reaction dynamics quantities obtained with the resulting PESs, since most tests of quantum chemistry methods in the literature are done at stationary points.

Another complication is that common electronic structure methods are robust only at geometries near equilibrium, while a proper sampling of the configuration space may demand potential energies at highly strained geometries where common coupled-cluster (CC) and Hartree–Fock (HF) methods may fail outright or return wildly incorrect energies that threaten to poison the fitting set. Finding electronic structure methods that are both feasible to use for automated PES development and robust enough is an open research problem.

With the use of sufficiently robust electronic structure methods and an adequate method for sampling the configuration space, it should be possible to create a computational protocol for the fully automated development of PESs suitable for reaction dynamics, without having to know the stationary points of the system beforehand. How exactly such a protocol would look like, and what is the best way to develop high-dimensional reactive PESs is an open question.

The $CH_3OH + \cdot OH$ reaction is of significant interest for combustion-, atmospheric-, and astrochemistry but previous studies have focused almost exclusively on the formation of $\cdot CH_2OH$ and $CH_3O\cdot$, and a comprehensive study that treats all stationary points and plausible products with the same high-accuracy method was yet to be published.

II. Methods

To probe how the reaction dynamics quantities are affected by the quantum chemistry approximations, we have computed new potential energies for the fitting set of a previously developed $CH_3I + F^-$ PES with 20 electronic structure method/basis set combinations: HF/DZ, HF/TZ, HF-D3(BJ)/DZ, HF-D3(BJ)/TZ, MP2/DZ, MP2/TZ, MP2-F12/DZ, MP2-F12/TZ, CCSD/DZ, CCSD-F12b/DZ, CCSD(T)/DZ, CCSD(T)-F12b/DZ, OQVCCD(T)/DZ, B97-1/TZ, PBE0/TZ, PBE0-D3(BJ)/TZ, M06-2X/TZ, M06-2X-D3(0)/TZ, B2PLYP/TZ and B2PLYP-D3(BJ)/TZ, where DZ denotes the aug-cc-pVDZ basis set and TZ denotes the aug-cc-pVTZ basis set. Using the 20 new PESs, we ran a total of ~10M quasi-classical trajectories (QCT), enabling us to analyze the differences in reactive cross sections, scattering angle distributions and product internal energy distributions.
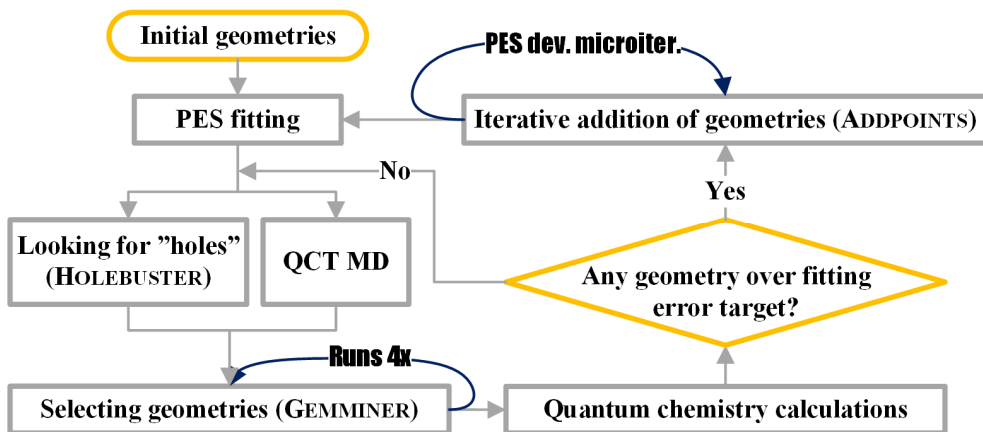
Figure 1 Simplified operational flowchart of the ROBOSURFER program system.

To reduce the time and labor required for creating a fitted PES for systems of ≥ 6 atoms the development of the ROBOSURFER program system (Figure 1) was begun, with the goal of writing new pieces of C++ software and combining them with existing Fortran 90 programs into a tool that automates the creation of new fitted PESs. Early versions of ROBOSURFER were then used to create PESs for the $CH_3Br + F^-$ reaction as a proof-of-concept, the $C_2H_6 + \cdot Cl$ reaction to test if QCT can match the experimental HCl rotational distribution, and the $C_2H_5Cl + F^-$ reaction to explain the competition between S_N2 and E2 reactivity and better interpret experimental data.

The $CH_3Br + F^-$ PES was developed by first running ROBOSURFER and using the DF-MP2-F12/TZ level of theory, then reselecting which of the geometries that have had their true potential energy computed in the first step should be included in the fitting set, and finally recomputing the energies of this final fitting set at the CCSD(T)-F12b/TZ level. The $C_2H_6 + \cdot Cl(^2P_{3/2})$ PES was developed by first running ROBOSURFER with RMP2/DZ, then recomputing the energies of the fitting set using a composite method that combines UCCSD(T)-F12b/DZ with an RMP2-F12 DZ/TZ basis correction and a spin-orbit (SO) contribution from an MRCI(5, 3) to approximate the SO ground state, and finally continuing to run ROBOSURFER with this composite $ab\ initio$ method. The $C_2H_5Cl + F^-$ PES was developed first at the DF-MP2-F12/DZ level, then with a composite method consisting of the CCSD(T)-F12b/AVDZ energy and an MP2-F12 DZ/TZ basis correction.

To find a way to resolve the problem of wildly incorrect energies being returned by the CCSD(T)-F12b method during the development of the $CH_3I + OH^-$ PES, we have examined 17 of the fitting set geometries where the CCSD(T)-F12b/DZ energy is lower than the MP2/DZ energy by >50 kcal/mol with 15 more quantum chemistry methods: HF/DZ, MP2-F12/DZ, MP2/TZ, MP2-F12/TZ, DF-MP2-F12/TZ, BCCD/DZ, BCCD(T)/DZ, BCCD(T)/TZ, OQVCCD/DZ, OQVCCD(T) /DZ, CCSD/DZ, CCSD-F12b/DZ, CCSD-F12b/TZ, CCSD(T)/DZ, and CCSDT/DZ.

To resolve the problem of HF convergence failures and incorrect HF energies seen for the $CH_3OH + \cdot OH$, $C_2H_6 + \cdot F$ and $CH_3NH_2 + \cdot Cl$ systems, the ManyHF method was implemented as a MOLPRO input script that contains an empirically determined minimal subset of preliminary HF and DFT computations that was found to not return incorrect energies in the reactant approach regions of the three tested systems. The test geometries were generated by randomly reorienting and distorting the approaching reactants, and then removing any excessively similar geometries.

The new $CH_3Cl + F^-$ PES was developed using the latest version of ROBOSURFER at the ManyHF-BCCD/aug-cc-pVD(+d)Z level, with a focus on only using information about the system that would be available in the setting of fully automated PES development.

The survey of the stationary points and products of the $CH_3OH + \cdot OH$ reaction used geometry optimizations and harmonic frequency computations at the ManyHF-UCCSD(T)-F12b/TZ level. These were followed by high-accuracy energy computations with a composite method that combines a CCSD(T) energy very close to the complete basis set limit with CCSDT(Q) and SO contributions, as well as corrections for core electron correlation and scalar relativistic effects.

Most quantum chemical computations were performed using MOLPRO 2015. The development of the new $CH_3Cl + F^-$ PES used MOLPRO 2023, all UHF-UCCSD(T) and post-(T) energies were computed using the MRCC package. The D3 contributions were computed with the DFT-D3 program. For Br and I atoms, the ECP10MDF and ECP28MDF effective core potentials were used respectively, with the aug-cc-pVnZ-PP basis sets. Open-shell energies were computed with an ROHF reference unless otherwise indicated. QCT simulations were carried out using the QCT code available in the research group. Most trajectories were analyzed using traditional project-specific tools written in Fortran 90 or C++, the $CH_3Br + F^-$ reaction probabilities and cross sections were extracted using a new universal trajectory analysis code written in C++.

III. Results
T1. I have recomputed the fitting set of the previous $CH_3I + F^-$ PES at 20 theoretical levels. Reaction dynamics results confirm that DFT and MP2 methods sufficiently fast for direct dynamics can cause significant inaccuracies. The most economical method that results in an accurate PES is CCSD(T)-F12b/aug-cc-pVDZ(-PP).

Direct dynamics does not require the construction of fitted PESs, but it is only feasible with theoretical levels that have a low computational cost: DFT and MP2 methods with small basis sets. Our computations have revealed that an accurate treatment of electron correlation and an effective basis set size of triple-ζ are both required for reliably accurate dynamics results. MP2/DZ S_N2 cross sections are 20-30% too large due to basis set incompleteness, while the H^+ abstraction cross sections are less than

half of the MP2/TZ results. The MP2 electron correlation approximation itself also causes the S_N2 cross sections to deviate from the more accurate CCSD(T) by 35-40%, demonstrating that using MP2 yields inaccurate dynamics results.

All tested DFT functionals yield exaggerated S_N2 reactivity, by a factor of ~2.5 in the worst case, which is attributable to anomalously high reaction probabilities in high-impact-parameter collisions. Alarmingly, the accuracy of the S_N2 ICSs obtained with a given functional is found to be inversely correlated with the functional's overall stationary-point accuracy. Although M06-2X/TZ performs reasonably well for $CH_3I + F^-$, no clear pattern emerges that could guide future research towards selecting the best functional for a given system, making it difficult to recommend DFT for computing accurate reaction dynamics quantities. Surprisingly, adding D3 dispersion has minimal effect on the DFT-based dynamics results.

Explicitly correlated F12 methods generally yield TZ-quality dynamics results with the DZ basis. Both the MP2-F12 and CCSD(T)-F12b results suggest that there would be little benefit to using basis sets larger than TZ for reaction dynamics and that CCSD(T)-F12b/DZ can be recommended.

T2. I have developed the ROBOSURFER program system, which automates the selection of geometries required for fitting high-dimensional PESs, and greatly reduces the human labour needed. The reaction dynamics results obtained using PESs developed with ROBOSURFER match experimental data well, for multiple systems. These PESs have made it possible for theory to both explain and complement measurements for systems larger than 6 atoms.

ROBOSURFER automates the iterative refinement of fitted PESs, as shown in Figure 1. Starting from some initial set of geometries a preliminary PES can be fitted, and the cycle that first uses the current PES to quickly generate many new geometries through QCT and other means, then selects the most promising new geometries, runs the required quantum chemical computations, and finally selectively adds geometries to the fitting set, can be started. This cycle is repeated until the configuration space is adequately sampled. The core ideas of ROBOSURFER are that:

 A) PESs are best improved by adding geometries to the fitting set where the fitting error is currently high.
 B) PESs are usually inaccurate in regions of insufficient sampling. Therefore, dissimilarity to the geometries already in the fitting set is a predictor of high fitting error.
 C) The most promising geometries are dissimilar but not too dissimilar to the fitting set.

ROBOSURFER is fitting method independent, no part of the geometry selection logic depends on the specifics of the fitting method, nor does ROBOSURFER demand un-

certainty estimates from the fitting method. ROBOSURFER is parallelized, and incorporates multiple heuristics to reduce the number of quantum chemistry computations required, such as explicitly searching for unphysical PES minima with HOLEBUSTER (a semi-local optimizer) and avoiding geometries close to geometries that have previously had convergence issues or returned a very high energy.

Since ROBOSURFER only adds geometries to the fitting set if their fitting error would otherwise be high, the automated PES development process also creates a large pool of geometries where the fitting error is known to be low, which considerably increases the confidence one can have in the quality of the resulting PESs.

ROBOSURFER has been successfully used for the development of over 20 PESs since its introduction, many of which were at the frontier of using fitted PESs for reaction dynamics at the time of publication. These PESs would have been extremely difficult to develop with the mostly manual methods used before ROBOSURFER, demonstrating that automated PES development is feasible for larger and more complicated systems and that ROBOSURFER is effective.

These high-fidelity surfaces enabled us to achieve major successes in reproducing and explaining experimental results. The $C_2H_5Cl + F^-$ PES enabled us to not only match experimental data but complement them. Due to the experimental limitation of only detecting charged products, it is not possible to reliably disentangle the contributions of the S_N2 and E2 reactions, and analyzing the experimentally available sum of contributions can sometimes even be misleading. With the required PES being available thanks to ROBOSURFER, theory can distinguish these reactions trivially, and reveal the missing pieces to the puzzle that experiment cannot see.

T3. Using ROBOSURFER, we have successfully developed a new PES for the $C_2H_6 + \cdot Cl(^2P_{3/2})$ reaction. QCT simulations ran with this PES yield a HCl rotational excitation distribution that agrees well with experimental data. The inaccuracy of previous QCT results in the literature stemmed primarily from the potentials used, not the QCT method.

Reactions between small alkanes and atoms have a long history of study, as their relative simplicity can allow a step-by-step explanation of reactions at the atomic level and can further a better understanding of the fundamental rules of chemical reactivity, such as the Polanyi rules. One of the experimentally accessible quantities is the rotational excitation distribution of the HCl product, and for $C_2H_6 + \cdot Cl(^2P_{3/2})$ all previous direct and PES-based QCT simulations yielded distributions that were too hot, leading to some suggesting that this may be an inherent limitation of the QCT approximation.

Our simulations show that this is not the case: using the new PES developed with ROBOSURFER we obtain a cold J-distribution that matches the experimental data al-

most quantitatively, resolving a nearly 25-year disagreement between theory and experiment and pointing to fitting errors and the use of inadequate quantum chemical methods as the sources of error in previous studies.

T4. Large negative errors in the (T) component of CCSD(T) energies at the extreme geometries demanded by automated PES development may derail PES development. A (T) contribution computed with BCCD(T) is more robust and composite methods using it meet the demands of automated PES development better.

We discovered that CCSD(T) can easily violate an implicit assumption of automated PES development: that the quantum chemistry method can be queried to obtain a valid potential energy at any arbitrary geometry. Occasional convergence failures, where no energy is returned, are tolerable but substantially incorrect energies can easily poison a fitting set, especially anomalously low energies. Unfortunately, CCSD(T) can return anomalously low energies for some geometries, which became untenable during the development of the $OH^- + CH_3I$ PES, when CCSD(T) energies fell below the much more robust CCSDT energies by up to 107 kcal/mol.

These spurious energies are attributable to the non-variational failure of the (T) approximation in CCSD(T) that may happen if a covalent bond is highly stretched. We find that the BCCD(T) Brueckner CC method can compute reasonable (T) contributions even at these geometries, and that a composite method combining the CCSD-F12b energy with the (T) contribution from BCCD(T) is substantially more robust than CCSD(T)-F12b, without giving up the lowered basis set error of F12 methods. This composite method only incurs a moderate increase in computational cost, and has since been successfully used for the development of over 7 PESs.

T5. Traditional Hartree–Fock methods are often incapable of reliably converging to the lowest energy solution for doublet systems, leading to unacceptable errors in post-HF energies and derailing automated PES development. I have developed the ManyHF method, which enhances the robustness of HF and post-HF computations by searching for the lowest-energy HF solution belonging to a given geometry.

The single-reference electronic structure methods practical for PES development generally rely on the HF reference to be a reasonable approximation of the exact ground-state wavefunction, and when this is not met their accuracy may be severely degraded. This may happen not only in cases where the molecular system has a genuine multireference character, but also in cases of HF misconvergence, where the HF solver algorithm returns an unstable HF solution, or even worse: a stable higher-energy solution.

I have found that the three doublet systems $CH_3OH + \cdot OH$, $C_2H_6 + \cdot F$ and $CH_3NH_2 + \cdot Cl$ all suffer severely from both HF non- and misconvergence using standard SCF (self-consistent field) methods, leading to erratic MP2 and CCSD(T)-F12b energies. The core idea of the ManyHF method is a global optimization strategy that first uses

various empirical tricks to create more diverse sets of initial orbitals, then runs multiple instances of the desired HF computation which differ both in the initial orbitals and the SCF algorithm being used, and finally selects the HF wavefunction with the lowest energy, which then can be used in post-HF computations.

Tests on the three aforementioned systems demonstrate that ManyHF finds better ROHF solutions and avoids non-convergence much more often than the default ROHF solver, without requiring any source code changes in MOLPRO or using exotic SCF solvers like semidefinite optimization or SCF-metadynamics. This is expected to extend the practical applicability of CCSD(T)-F12 and other single-reference methods to systems with moderately difficult electronic structure, especially when it comes to reactions involving radicals. ManyHF has successfully been used in the development of over 5 PESs.

T6. If the electronic structure method used is sufficiently robust and does not return wildly inaccurate energies at extreme geometries, then PES development may be conducted with ROBOSURFER without any foreknowledge of the products and stationary points. This opens the way towards full automation and the automated discovery of stationary points.

The ROBOSURFER program system has been considerably upgraded since its first versions, to fix various issues and limitations discovered through usage, make it more user-friendly, and to push towards the goal of fully automated PES development. I have implemented two new techniques to increase the flexibility of PIP-based fitting and counter the growth of the weighted RMS fitting errors of the fitting set: the gradual addition of 2-, 3- and 4-body extra monomials to the PIP fitting basis and the repeated global optimization of the handful of nonlinear parameters used in the fitting function over the course of PES development. The development of the new $CH_3Cl + F^-$ PES was started only from reactant-side geometries that could in principle be automatically generated without knowing anything about a system, not even what reactions might take place.

After extensive sampling of the configuration space using ROBOSURFER, these efforts have yielded a new PES for $CH_3Cl + F^-$ which has low fitting errors in the chemically relevant regions, as shown by both the low RMS fitting errors of the fitting set and the high-fidelity reproduction of reactant-side potential energy curves. Most importantly, this latest version of ROBOSURFER has managed to develop a PES that is correct at the stationary points of the system, even though the development process was only seeded with geometries generated from the reactants. Although some issues are yet to be overcome, particularly when it comes to improving the fitting fidelity reachable with the PIP method, it seems likely that future versions of ROBOSURFER could become able to develop full-dimensional global PESs as a fully automated and perhaps standardized computational protocol, at least if a sufficiently robust electronic structure method is feasible for the chemical system in question.

T7. I have conducted a comprehensive survey of the stationary points and plausible products of the $CH_3OH + \cdot OH$ reaction, using high-accuracy *ab initio* methods. According to my computations there are other thermodynamically favorable products besides $\cdot CH_2OH$ and $CH_3O\cdot$, such as methanediol and the hydroxymethoxy radical.

I have surveyed the configuration space of CO_2H_5 system, including not only the traditional minima and barriers of the $CH_3OH + \cdot OH$ reaction but also alternative barriers, conformational saddle points, product isomerization, product dissociation and some of the conceivable exotic products. Optimizing 29 geometries has revealed that a hitherto unknown stationary point exists in the reactant complex region. Furthermore, our optimizations support that the previously known reactant complex is nonsymmetric, resolving the disagreement between two recent publications.

The final results are in excellent agreement with 0 K reaction enthalpies from the ATcT database and often improve upon previous literature results. We confirm that the barrier height of $CH_3O\cdot$ formation is very sensitive to the electronic structure theory used, and that post-(T) correlation is essential for computing it accurately. Our ZPE-inclusive barrier heights for dissociating a H-atom from $\cdot CH_2OH$ and $CH_3O\cdot$ are only 16.04 and 10.31 kcal/mol above the reactants, suggesting that formaldehyde formation may be possible in reaction dynamics if $CH_3O\cdot$ and $\cdot CH_2OH$ form with a large amount of internal energy. For the formation of $CH_2(OH)_2 + \cdot H$ and $CH_2OHO\cdot + H_2$ we predict 0 K reaction enthalpies of −2.43 and −1.65 kcal/mol, respectively.

This, in combination with the possibility of H_2CO formation and isomerization between the two main products, suggests that the bimolecular collision dynamics of $CH_3OH + \cdot OH$ may be far more interesting than previously thought.

IV. List of publications
IV.A Publications covered in this thesis

1. **T. Győri**, B. Olasz, G. Paragi, G. Czakó: *Effects of the level of electronic structure theory on the dynamics of the F⁻ + CH₃I reaction*, J. Phys. Chem. A, 122, 3353 (2018) 10.1021/acs.jpca.8b00770 IF: 2.64

2. **T. Győri**, G. Czakó: *Automating the development of high-dimensional reactive potential energy surfaces with the ROBOSURFER program system*, J. Chem. Theory Comput., 16, 51 (2020) 10.1021/acs.jctc.9b01006 IF: 6.01

3. D. Papp, V. Tajti, **T. Győri**, G. Czakó: *Theory finally agrees with experiment for the dynamics of the Cl + C₂H₆ reaction*, J. Phys. Chem. Lett, 11, 4762 (2020) 10.1021/acs.jpclett.0c01263 IF: 6.48

4. D. A. Tasi, **T. Győri**, G. Czakó: *On the development of a gold-standard potential energy surface for the OH⁻ + CH₃I reaction*, Phys. Chem. Chem. Phys., 22, 3775 (2020) 10.1039/C9CP07007A IF: 3.68

5. J. Meyer, V. Tajti, E. Carrascosa, **T. Győri**, M. Stei, T. Michaelsen, B. Bastian, G. Czakó, R. Wester: *Atomistic dynamics of elimination and nucleophilic substitution disentangled for the F⁻ + CH₃CH₂Cl reaction*, Nat. Chem. 13, 977 (2021) 10.1038/s41557-021-00753-8 IF: 24.27

6. **T. Győri**, G. Czakó: *ManyHF: A pragmatic automated method of finding lower-energy Hartree–Fock solutions for potential energy surface development*, J. Chem. Phys., 156, 071101 (2022) 10.1063/5.0080817 IF: 4.40

7. **T. Győri**, G. Czakó: *A comprehensive benchmark ab initio survey of the stationary points and products of the OH· + CH₃OH system*, J. Chem. Phys., 158, 034301 (2023) 10.1063/5.0133978 IF: 3.10

IV.B Publications related to this thesis

1. G. Czakó, **T. Győri**, B. Olasz, D. Papp, I. Szabó, V. Tajti, D. A. Tasi: *Benchmark ab initio and dynamical characterization of the stationary points of reactive atom + alkane and S_N2 potential energy surfaces*, Phys. Chem. Chem. Phys., 22, 4298 (2020) 10.1039/C9CP04944D IF: 3.68

2. G. Czakó, **T. Győri**, D. Papp, V. Tajti, D. A. Tasi: *First-principles reaction dynamics beyond six-atom systems*, J. Phys. Chem. A, 125, 2385 (2021) 10.1021/acs.jpca.0c11531 IF: 2.94

3. V. Tajti, **T. Győri**, G. Czakó: *Detailed quasiclassical dynamics of the F⁻ + CH₃Br reaction on an ab initio analytical potential energy surface*, J. Chem. Phys., 155, 124301 (2021) 10.1063/5.0065209 IF: 4.30

4. P. Tóth, T. Szűcs, **T. Győri**, G. Czakó: *Dynamics of the Cl + CH₃CN reaction on an automatically-developed full-dimensional ab initio potential energy surface*, J. Chem. Phys., 10.1063/5.0220917. IF: 3.1

Hungarian Science Bibliography (MTMT) identifier: 10065009
Cumulative impact factor of the publications covered in this thesis: 50.58.
Cumulative impact factor of all publications: 64.6.

V. Talks and posters

V.A International conference talks and posters

1. T. Győri, G. Czakó: *Automated PES development with ROBOSURFER and ManyHF: active learning demands robust electronic structure theory and implementation*, New directions in molecular scattering Faraday Discussion, Edinburgh (UK), 08.05.2024. (poster)

2. T. Győri, G. Czakó: *Automated development of PESs via active learning: a real-world stress test of electronic structure theories and implementations?*, 17th International Congress of Quantum Chemistry, Bratislava (SK), 27.06.2023. (poster)

3. T. Győri, D. A. Tasi, V. Tajti, D. Papp, G. Czakó: *Tools for automated PES development: Robosurfer and ManyHF*, XVI. Quantum Reactive Scattering Workshop, Balatonföldvár (HU), 05.09.2022. (talk)

4. T. Győri, D. A. Tasi, V. Tajti, D. Papp, G. Czakó: *Towards automated potential energy surface development with Robosurfer and ManyHF*, Molecular Interactions and Dynamics Gordon Research Conference, Easton (US), 11-12.06.2022. (poster & talk)

5. T. Győri: *Introduction to the quasiclassical trajectory method and reactive potential energy surface fitting; The ManyHF method*, 3rd YoungCAS workshop on Global SCF Optimization, Oslo (NO), 22.06.2022. (invited talk)

6. T. Győri, G. Czakó: *Automated potential energy surface development: Application to the $F^- + CH_3Br$ system*, XXVIIIth International Symposium on Molecular Beams, Edinburgh (UK), 22.06.2019. (poster)

V.B National conference talks

1. T. Győri, G. Czakó: *Towards automated potential energy surface development with Robosurfer and ManyHF*, Mátrafüred, Meeting of the MTA Material and Molecular Structure Working Group, 22.10.2022.

2. T. Győri, G. Czakó: *Jobb Hartree–Fock megoldások keresésének automatizálása a ManyHF módszerrel*, Szeged, KeMoMo-QSAR Symposium, 02.06.2018.

3. T. Győri, G. Czakó: *Potenciálisenergia-felületek fejlesztésének automatizálása*, Veszprém, Meeting of the MTA Reaction Kinetics and Photochemistry Working Group, 08.11.2018.

4. T. Győri, G. Czakó: *Potenciálisenergia-felületek fejlesztésének automatizálása*, Szeged, XLI. Chemical Lecture Days, 15.10.2018.

5. T. Győri, G. Czakó: *A $F^- + CH_3Br$ reakció potenciális energia felületének automatikus fejlesztése*, Szeged, KeMoMo-QSAR Symposium, 25.05.2018.