



UNIVERSITÀ DEGLI STUDI DI MILANO



Constructing PIP potential energy surfaces for semiclassical vibrational spectroscopy calculations

Riccardo Conte

VISTA, June 26th, 2024

Acknowledgments

Main Collaborators (SC spectroscopy)



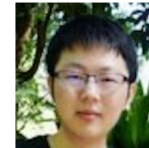
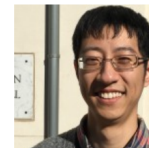
Michele Ceotto (Milan Univ.)
Chiara Aieta (Milan Univ. and Princeton Univ.)
Marco Cazzaniga (Milan Univ.)
Giacomo Botti (Milan Univ.)
Cecilia Lanzi (Milan Univ.)
Giacomo Mandelli (Milan Univ.)
Davide Moscato (Milan Univ.)



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Main collaborators (PIP PESS)

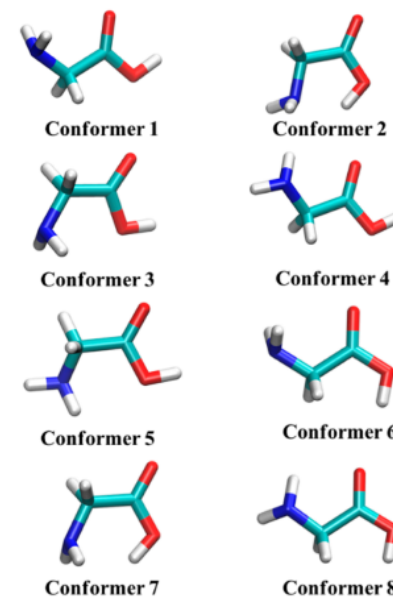
Joel M. Bowman (Emory Univ.)
Paul L. Houston (Cornell Univ. and Georgia Tech)
Apurba Nandi (Univ. of Luxembourg)
Chen Qu (NIST)
Qi Yu (Fudan Univ.)
Priyanka Pandey (Emory Univ.)



Talk Outline

1. Building potential energy surfaces with permutationally invariant polynomials (PIPs)

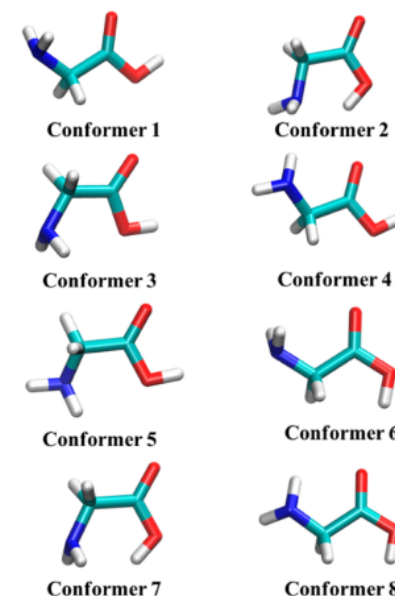
- Theory of (PIPs): Fragmentation; Many-body Approach; Pruning
- Accuracy and performance comparison to other ML methods
- Improving the level of a PIP PES



Talk Outline

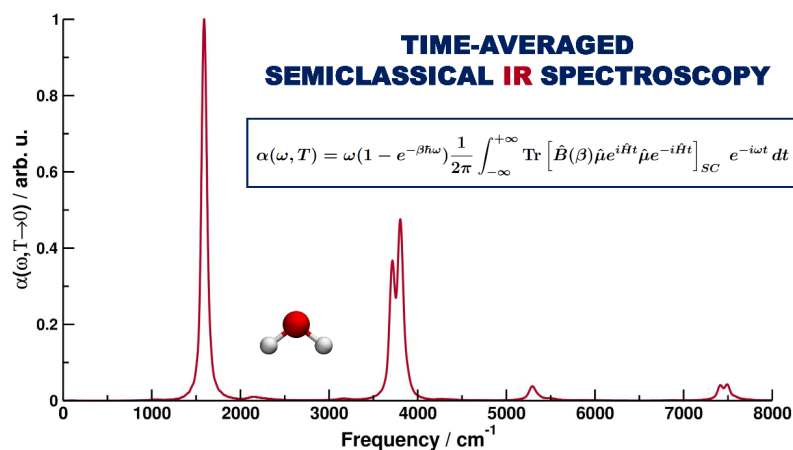
1. Building potential energy surfaces with permutationally invariant polynomials (PIPs)

- Theory of (PIPs): Fragmentation; Many-body Approach; Pruning
- Accuracy and performance comparison to other ML methods
- Improving the level of a PIP PES



2. Semiclassical (SC) vibrational Spectroscopy

- Theory and advances in SC vibrational spectroscopy
- Accuracy and importance of SC spectroscopy
- A new time-averaged SC IR spectroscopy approach



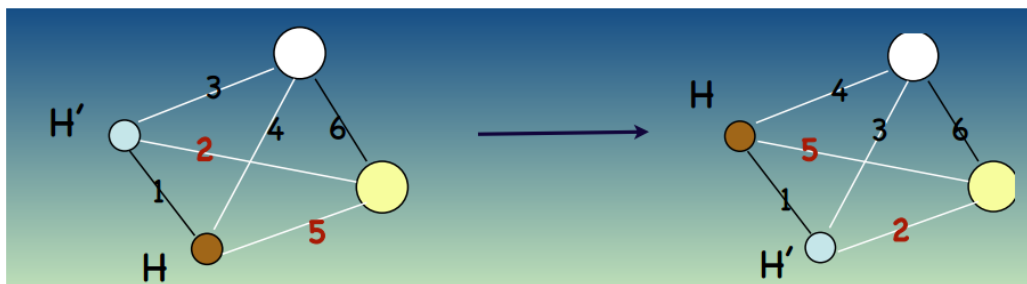
Permutationally Invariant Polynomials (PIPs)

Generic polynomial expression for the potential energy

$$V = \sum_{a+b+c+d+e+f \leq N} C_{abcdef} [y_{12}^a y_{13}^b y_{14}^c y_{23}^d y_{24}^e y_{34}^f]; y_{ij} = \exp(-r_{ij} / \lambda)$$

C_{abcdef} Linear coefficients to be fitted to *ab initio* data

N is maximum polynomial order; λ is usually chosen in the range 2-3 Bohr



No permutation invariance!

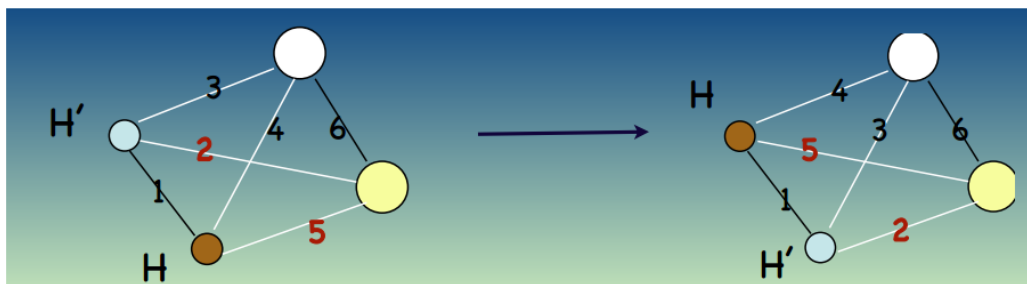
Permutationally Invariant Polynomials (PIPs)

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No permutation invariance!

PIP expression for the potential energy

$$V = \sum_{n_1 + \dots + n_6 \leq N} c_n \hat{S}\{y_1^{n_1} y_2^{n_2} y_3^{n_3} y_4^{n_4} y_5^{n_5} y_6^{n_6}\}$$

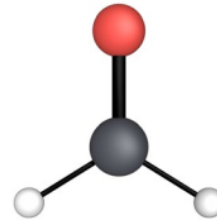
$$V(r_1, \dots, r_6) = \sum_{n_1, \dots, n_6} C_{n_1 \dots n_6} y_1^{n_1} y_6^{n_6} (y_2^{n_2} y_3^{n_3} y_4^{n_4} y_5^{n_5} + y_2^{n_5} y_3^{n_4} y_4^{n_3} y_5^{n_2})$$

Permutationally Invariant Polynomials (PIPs)

PIP expression for the potential energy

$$V = \sum_{n_1 + \dots + n_6 \leq N} D_n \hat{S}\{y_1^{n_1} y_2^{n_2} y_3^{n_3} y_4^{n_4} y_5^{n_5} y_6^{n_6}\}$$

An easy example: Formaldehyde



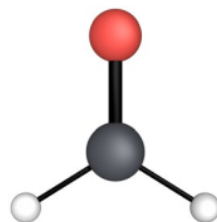
	H1	H2	C	O
H1		r_1	r_2	r_3
H2	r_1		r_4	r_5
C	r_2	r_4		r_6
O	r_3	r_5	r_6	

Permutationally Invariant Polynomials (PIPs)

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H2	r_1		r_4	r_5
C	r_2	r_4		r_6
O	r_3	r_5	r_6	

Some of the PIPs

$$p(0) = 1$$

$$p(1) = \exp(-r_1/a)$$

$$p(2) = \exp(-r_2/a) * \exp(-r_4/a)$$

$$p(3) = \exp(-r_3/a) * \exp(-r_5/a)$$

$$p(4) = \exp(-r_6/a)$$

$$p(5) = \exp(-r_2/a) + \exp(-r_4/a)$$

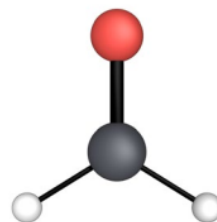
$$p(6) = \exp(-r_3/a) + \exp(-r_5/a)$$

Permutationally Invariant Polynomials (PIPs)

PIP expression for the potential energy

$$V = \sum_{n_1 + \dots + n_6 \leq N} D_n \hat{S}\{y_1^{n_1} y_2^{n_2} y_3^{n_3} y_4^{n_4} y_5^{n_5} y_6^{n_6}\}$$

An easy example: Formaldehyde



	H1	H2	C	O
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Some of the PIPs

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$$p(5) = \exp(-r_2/a) + \exp(-r_4/a)$$

$$p(6) = \exp(-r_3/a) + \exp(-r_5/a)$$

No. PIPs vs Max Pol Order

max. polynomial order	2	3	4	5	6	7	8	9
No. polynomials	18	50	120	256	502	918	1589	2625

Available Software

PESPIP: P.L. Houston, C. Qu, Q. Yu, R. Conte, A. Nandi, J.K. Li, J.M. Bowman *J. Chem. Phys.* **158**, 044109 (2023); <https://doi.org/10.1063/5.0134442>

Permutationally Invariant Polynomials (PIPs)

PIP notation is of type $A_l B_m C_n \dots$, where A, B, C, ... are atom types, and l, m, n indicates the permutation order for the corresponding atom.

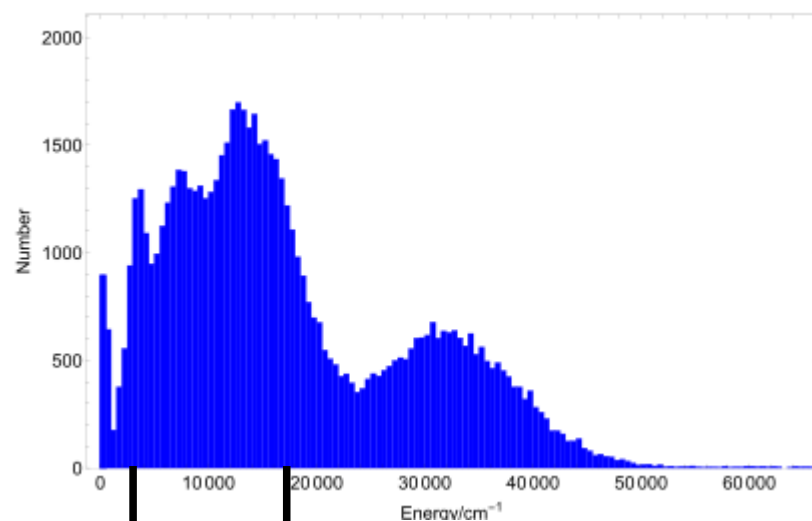
Number of PIPs depending on molecule permutational symmetry and maximum polynomial order

	5	6	7	8
A_2B	34	50	70	95
A_3B	103	196	348	590
ABCD	462	924	1716	3003
A_3B_2	364	889	2022	4343
A_2B_2C	904	2304	5416	11910
ABCDE	3003	8008	19448	43758

- No. polys increases rapidly with number of atoms
- No. polys decreases if symmetry is higher, but polys are slower to evaluate

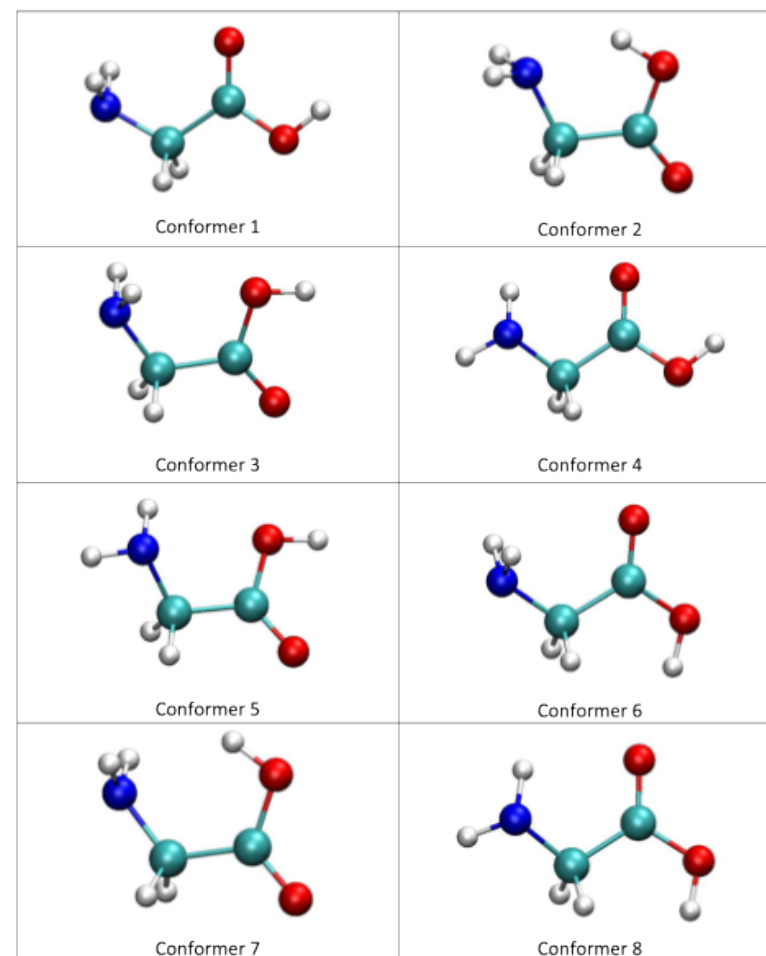
A PES for glycine ($A_5B_2C_2D$)

- The dataset should be designed according to the foreseen applications. Quantum simulations require sampling of high energies.
- For glycine about 70,000 *ab initio* energies and gradients have been calculated at DFT/B3LYP/aVDZ level and fitted by means of 22,250 PIPs (fit order 4)



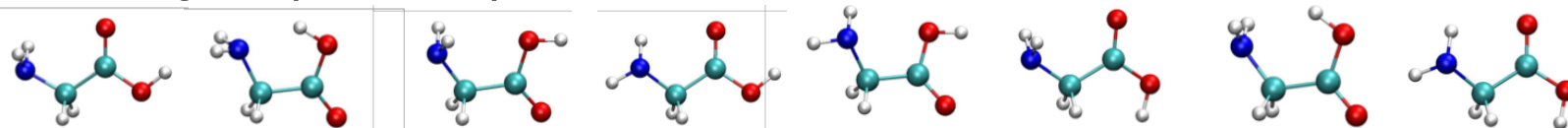
Max of room T
sampling

Zero point energy




A PES for glycine

Electronic energies (kcal/mol)

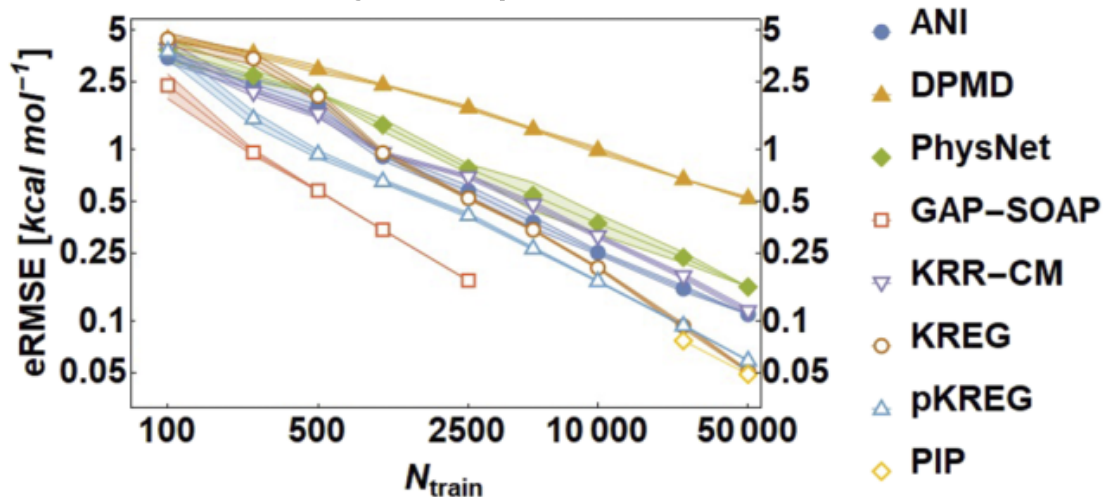
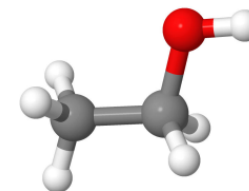


	Conf 1	Conf 2	Conf 3	Conf 4	Conf 5	Conf 6	Conf 7	Conf 8
PES	0.00	0.59	1.65	1.29	2.70	4.92	5.84	6.22
B3LYP	0.00	0.58	1.64	1.27	2.61	4.91	5.84	6.25
CCSD (T)	0.00	0.68	1.73	1.23	2.62	4.80	5.89	6.06

- Harmonic frequencies: MAE $\sim 6 \text{ cm}^{-1}$
 - 8 conformers and 15 saddle points identified
 - Diffusion Monte Carlo zero-point energy simulations
- 
- The 8 conformers can be group into 4 pairs of asymmetric double wells

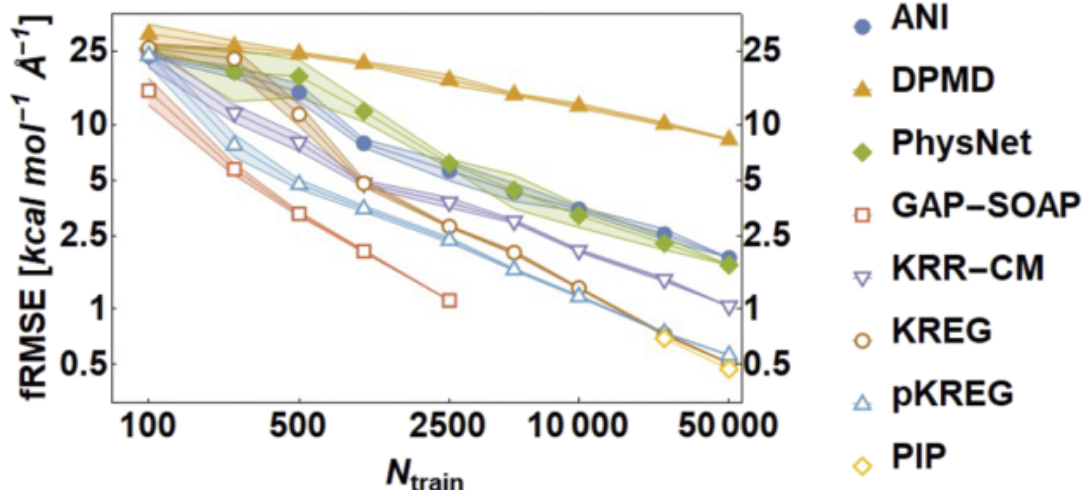
Accuracy and efficiency of a PIP PES

- Comparison of accuracy and speed between several ethanol PES
- 14,752 PIPs (fit order 4)
 - Accuracy comparison



- cpu time comparison for 20,000 energy and 20,000 force calls. Training size needed for eRMSE = 0.1 kcal/mol

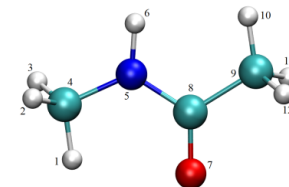
	Training Size	cpu Time (s)
pKREG	25,000	227
KRR-CM	50,000	508
GAP-SOAP	2,500	3611
s-GDML	1,000	25
ANI	50,000	26
Physnet	50,000	300
PIP	25,000	2.3



What About Larger Systems?

● The fragmentation technique

- identify atoms which are unlikely to permute
- divide the molecule into overlapping subsystems
- eliminate repeated polynomials

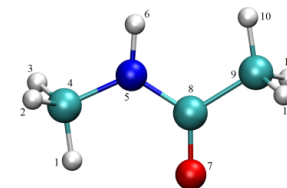


N-methyl acetamide

What About Larger Systems?

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N-methyl acetamide

Training dataset made of 3000 energies and 3000 gradients (DFT-B3LYP/cc-pVDZ)
Coefficients are linear, so least squares fitting is employed

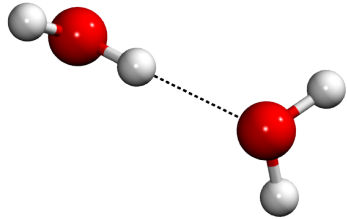
Fit Order	3	3	3
No. Frags	1	2	3
RMS (energy)*	26.8	34.3	148.9
RMS (gradient)**	54.7	67.4	171.8
Time***	6.611	2.450	0.830

* cm^{-1} ; ** $\text{cm}^{-1}/\text{Bohr}$; *** s, evaluation of 3000 energies and gradients on a 2.7 GHz cpu



What About Larger Systems?

- The many-body expansion and pruning of polynomials



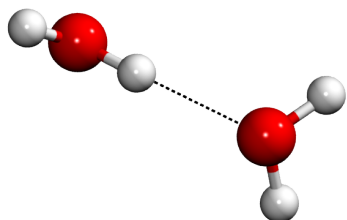
$$V = V_{1b} + V_{2b} + V_{3b} + \dots$$

$$V(A \cdots B) = V_{1b}(A) + V_{1b}(B) + V_{2b}(A \cdots B)$$

Some of the polynomials are not returning the correct long-range vanishing 2-body interaction

What About Larger Systems?

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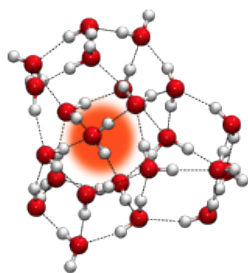
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Some of the polynomials are not returning the correct long-range vanishing 2-body interaction



Those polynomials are eliminated from the fitting basis set. Accuracy maintained, smaller training dataset



q-AQUA, MB-pol, q-AQUA-pol, MB-pol(2023) are all very accurate PIP potentials for water.

Q.Yu, C. Qu, P.L. Houston, **R. Conte**, A. Nandi, J.M. Bowman *J. Phys. Chem. Lett.* **13**, 5068 (2022)

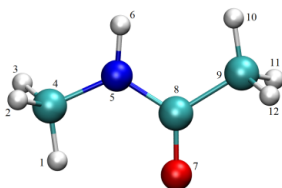
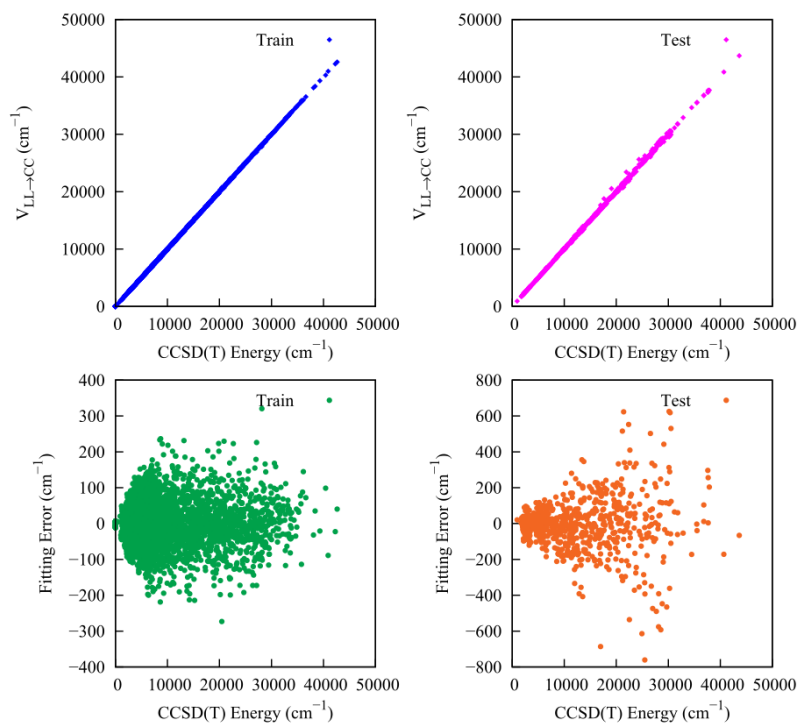
Q.Yu, C. Qu, P.L. Houston, **R. Conte**, A. Nandi, J.M. Bowman *J. Chem. Theory Comput.* **19**, 3446 (2023)

Improving the Level of the PES

- It is possible to “correct” a low level (LL) PES by fitting a difference PES based on a high level, coupled cluster (CC) training set

$$V_{LL \rightarrow CC} = V_{LL} + \Delta V_{CC-LL}$$

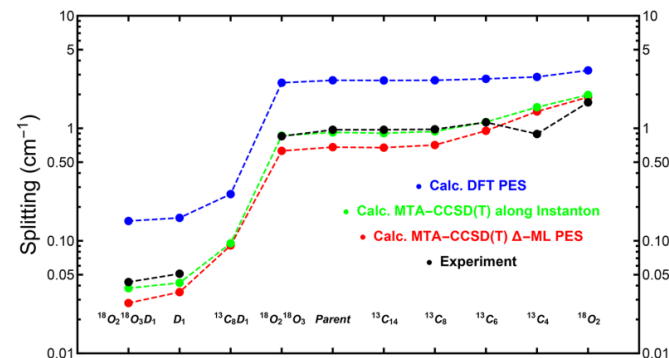
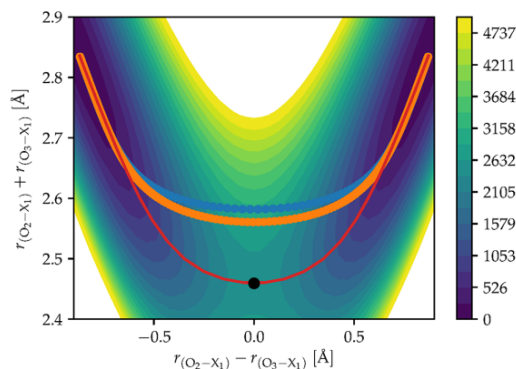
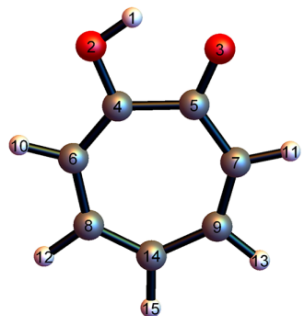
Δ - machine learning technique. About 6000 energies and gradients at DFT-B3LYP/cc-pVDZ level for N-methyl acetamide (V_{LL}). About 4700 energies at CCSD(T)/aug-cc-pVDZ for the Δ surface.



Application to torsional barriers

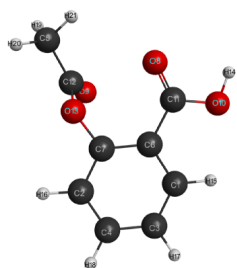
<i>trans</i> -NMA	CH ₃ -NH	CH ₃ -CO
DFT PES	256	37
Δ -ML PES	34	74
CCSD(T)	42	103
<i>cis</i> -NMA	CH ₃ -NH	CH ₃ -CO
DFT PES	61	361
Δ -ML PES	153	366
CCSD(T)	148	303

A pair of recent applications of PIP PESs

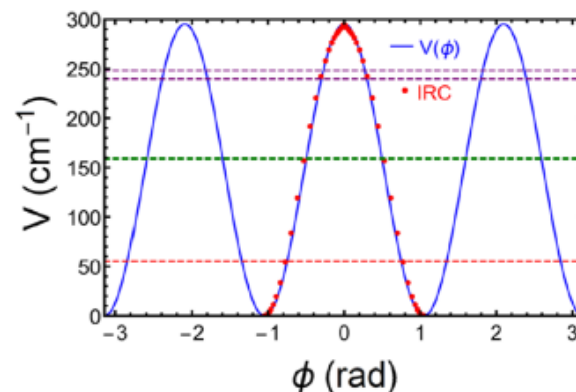
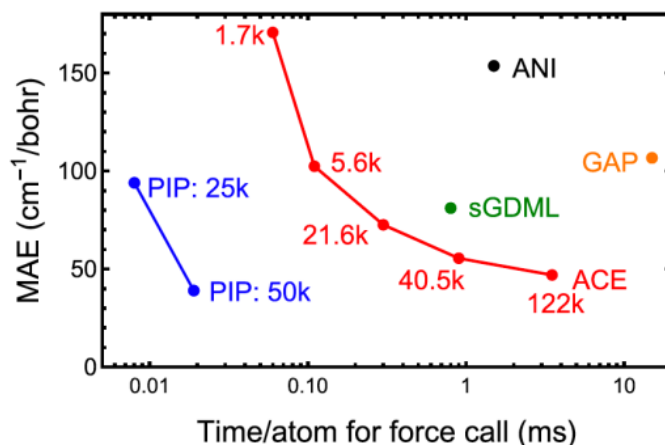


Δ - ML PES Calculation of H-transfer tunneling splitting with semiclassical instanton

A. Nandi, G. Laude, S.S. Khire, N.D. Gurav, C. Qu, **R. Conte**, Q. Yu, S. Li, P.L. Houston, S.R. Gadre, J.O. Richardson, F.A. Evangelista, J.M. Bowman *J. Am. Chem. Soc.* **145**, 9655 (2023).



DFT PES
MD17 dataset



P.L. Houston, C. Qu, Q. Yu, P. Pandey, **R. Conte**, A. Nandi, J.M. Bowman, S.G. Kukolich *J. Chem. Theory Comput.* **30**, 3008 (2024).

Semiclassical spectroscopy

- Power Spectra from Fourier transform of a survival amplitude

$$I(E) = \frac{1}{\pi\hbar} \text{Re} \int_0^{+\infty} dt e^{iEt/\hbar} \langle \Psi | \Psi(t) \rangle \quad |\Psi(t)\rangle = e^{-i\hat{H}t/\hbar} |\Psi\rangle$$

Semiclassical vibrational spectroscopy

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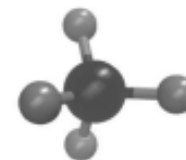
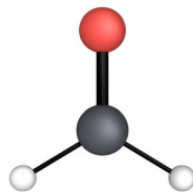
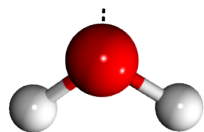
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- Semiclassical approximation to the propagator (Herman Kluk)

$$e^{-i\hat{H}t/\hbar} \approx \left(\frac{1}{2\pi\hbar} \right)^{N_{vib}} \int \int d\mathbf{p}_0 d\mathbf{q}_0 C_t(\mathbf{p}_0, \mathbf{q}_0) e^{iS_t(\mathbf{p}_0, \mathbf{q}_0)/\hbar} |\mathbf{p}_t, \mathbf{q}_t\rangle \langle \mathbf{p}_0, \mathbf{q}_0|$$

- Application to small molecules through Kaledin and Miller's time average

$$I(E) = \left(\frac{1}{2\pi\hbar} \right)^{N_{vib}} \int \int d\mathbf{p}_0 d\mathbf{q}_0 \frac{1}{2\pi\hbar T} \left| \int_0^T dt e^{i[S_t(\mathbf{p}_0, \mathbf{q}_0) + \phi_t(\mathbf{p}_0, \mathbf{q}_0) + Et]/\hbar} \langle \Psi | \mathbf{p}_t, \mathbf{q}_t \rangle \right|^2$$



Semiclassical vibrational spectroscopy

Application to small molecules through Kaledin and Miller's time average

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- Is it possible to perform SC spectroscopy on complex or larger systems?



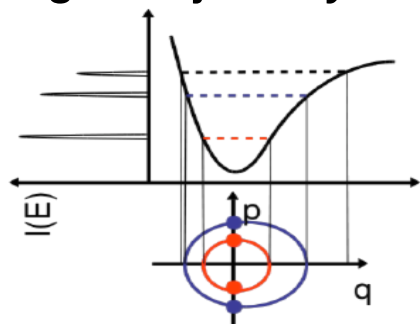
PES not always available

Need to collect a sensible spectroscopic signal

- How accurate is SC spectroscopy?
- Why performing SC spectroscopy instead of classical calculations?
- Is it possible to calculate SC IR spectra?

Semiclassical spectroscopy of larger systems

1. Single trajectory simulations (“on-the-fly” calculations) (**MC SCIVR**)



1A) Classical Trajectories with Tailored Energy

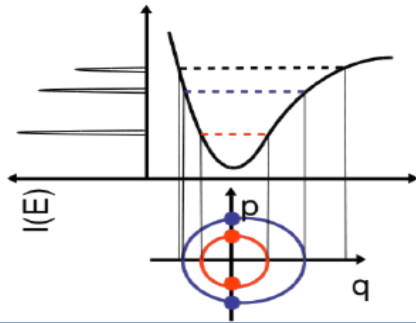
1B) Tailored Choice of Reference State

$$|\Psi\rangle = \sum_{i=1}^{N_{st}} \prod_{j=i}^{N_{vib}} \varepsilon_i(j) |p_{eq,j}^{(i)}, q_{eq,j}^{(i)}\rangle$$

M. Ceotto, S. Atahan, G. F. Tantardini, and A. Aspuru-Guzik *J. Chem. Phys.* **130**, 234113 (2009).

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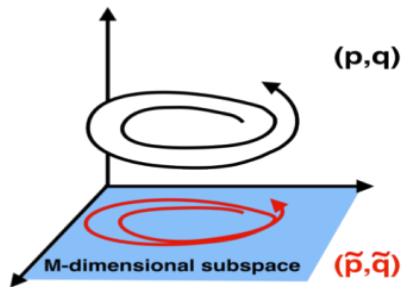


1A) Classical Trajectories with Tailored Energy

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$$|\Psi\rangle = \sum_{i=1}^{N_{st}} \prod_{j=i}^{N_{vib}} \varepsilon_i(j) |p_{eq,j}^{(i)}, q_{eq,j}^{(i)}\rangle$$

2. Projection on subspaces (sensible signals even from large systems) (**DC SCIVR**)



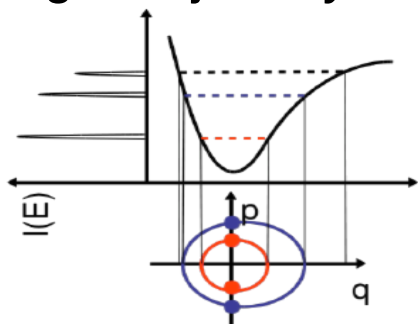
The semiclassical partial spectra are obtained from subspace-projected quantities, while the dynamics is full dimensional

$$\tilde{I}(E) = \left(\frac{1}{2\pi\hbar} \right)^M \int \int d\tilde{\mathbf{p}}_0 d\tilde{\mathbf{q}}_0 \frac{1}{2\pi\hbar T} \left| \int_0^T e^{\frac{i}{\hbar} [\tilde{S}_t(\tilde{\mathbf{p}}_0, \tilde{\mathbf{q}}_0) + Et + \tilde{\phi}_t]} \langle \tilde{\Psi} | \tilde{\mathbf{p}}_t, \tilde{\mathbf{q}}_t \rangle dt \right|^2$$

M. Ceotto, G. Di Liberto, and **R. Conte** *Phys. Rev. Lett.* **119**, 010401 (2017).

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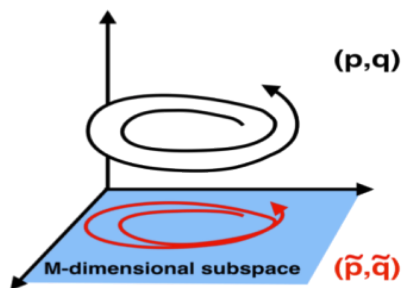


1A) Classical Trajectories with Tailored Energy

1B) Tailored Choice of Reference State

$$|\Psi\rangle = \sum_{i=1}^{N_{st}} \prod_{j=i}^{N_{vib}} \varepsilon_i(j) |p_{eq,j}^{(i)}, q_{eq,j}^{(i)}\rangle$$

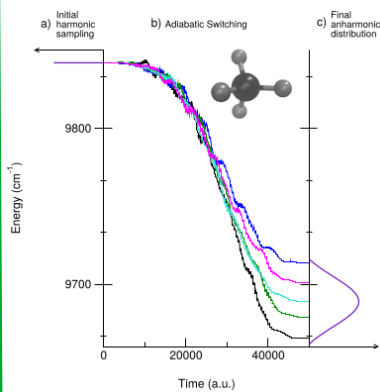
2. Projection on subspaces (sensible signals even from large systems) (**DC SCIVR**)



The semiclassical partial spectra are obtained from subspace-projected quantities, while the dynamics is full dimensional

$$\tilde{I}(E) = \left(\frac{1}{2\pi\hbar} \right)^M \int \int d\tilde{\mathbf{p}}_0 d\tilde{\mathbf{q}}_0 \frac{1}{2\pi\hbar T} \left| \int_0^T e^{\frac{i}{\hbar} [\tilde{S}_t(\tilde{\mathbf{p}}_0, \tilde{\mathbf{q}}_0) + Et + \tilde{\phi}_t]} \langle \tilde{\Psi} | \tilde{\mathbf{p}}_t, \tilde{\mathbf{q}}_t \rangle dt \right|^2$$

3. Adiabatic Switching (increase of precision and accuracy) (**AS SCIVR**)



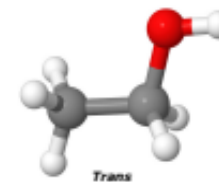
Preparing initial conditions upon switching on slowly the real Hamiltonian allows for full dimensional calculations of larger systems and better accuracy of results.

M. Ceotto, S. Atahan, G. F. Tantardini, and A. Aspuru-Guzik *J. Chem. Phys.* **130**, 234113 (2009).

M. Ceotto, G. Di Liberto, and **R. Conte** *Phys. Rev. Lett.* **119**, 010401 (2017).

R. Conte, L. Parma, C. Aieta, A. Rognoni, and M. Ceotto *J. Chem. Phys.* **151**, 214107 (2019).

Is semiclassical spectroscopy accurate?



Study of the vibrational frequencies of ethanol on a CCSD(T) analytical PES

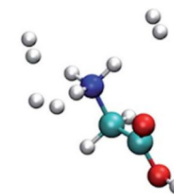
- Analytical surface at CCSD(T)-F12a/aug-cc-pVDZ level of theory constructed via Δ - machine learning starting from a PES at DFT level of theory.

	VCI (DMC)	AS SCIVR	EXPT		VCI	AS SCIVR	EXPT
ZPE	(17321)	17298	-	CH ₃ -adef''	1459	1456	1460
CO-str	1101	1088	1090	CH ₂ -sdef	1489	1481	1500
CH ₂ -rck	1160	1148	1166	CH ₂ -sstr	2811	2881	2888
COH-bnd	1251	1242	1241	CH ₂ -astr	2884	2888	2902
CH ₂ -twst	1276	1271	1275	CH ₃ -sstr	2937	2933	2922
CH ₃ -sdef	1370	1363	1367	CH ₃ -astr''	2977	2983	2987
CH ₂ -wag	1426	1420	1430	CH ₃ -astr'	2981	2986	2992
CH ₃ -adef'	1443	1440	1455	OH-str	3672	3676	3676
				MAE	13	7	-

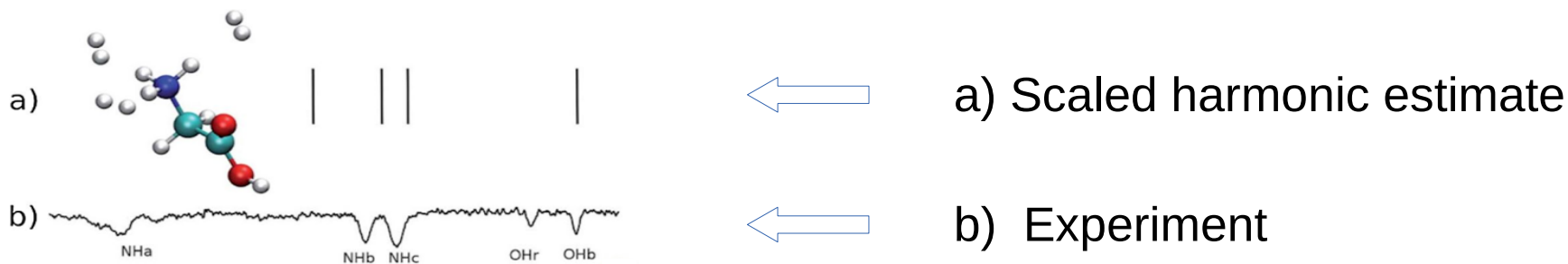
- AS SCIVR detects Fermi resonances and the zero point energy accurately



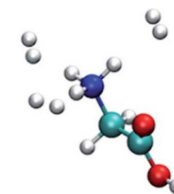
The importance of a quantum approach



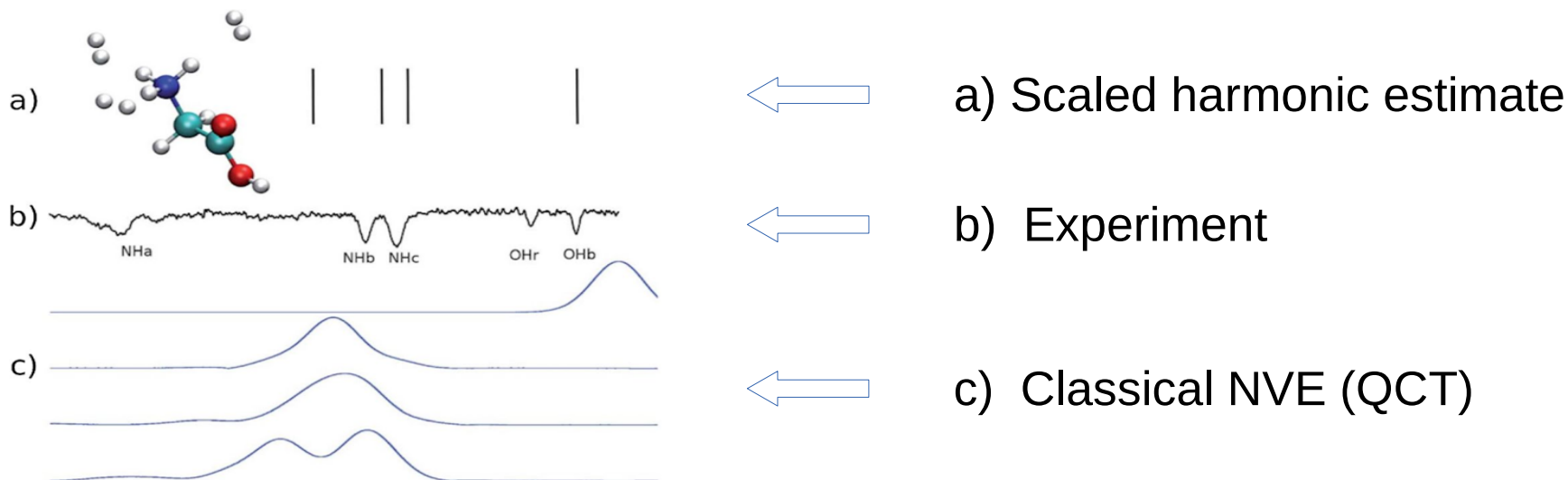
Calculation of high frequency fundamentals for H₂-tagged protonated glycine



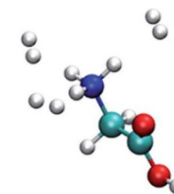
The importance of a quantum approach



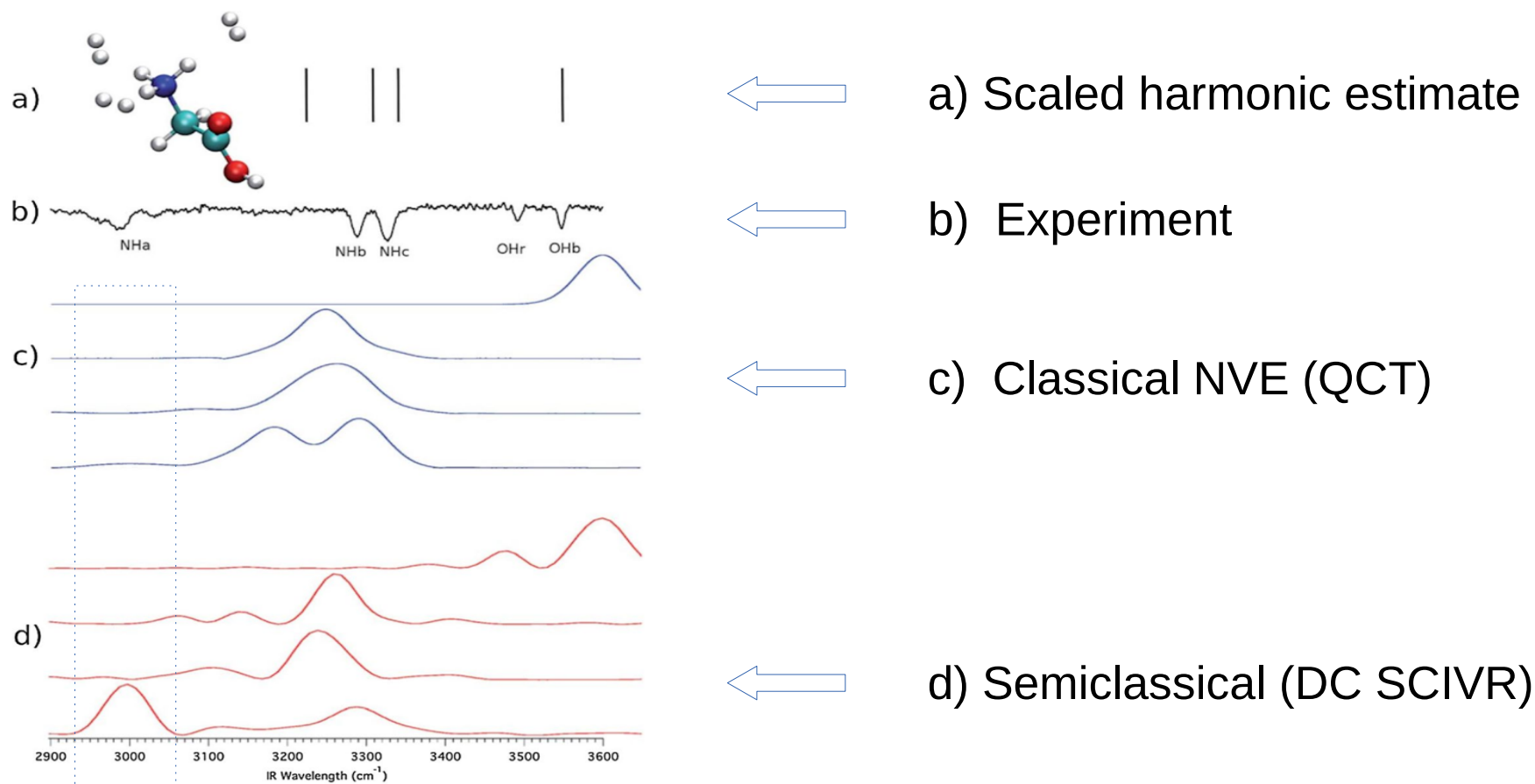
Calculation of high frequency fundamentals for H₂-tagged protonated glycine



The importance of a quantum approach

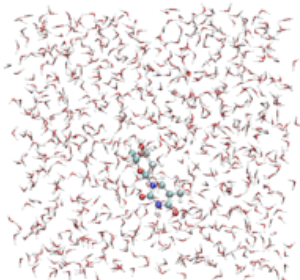


Calculation of high frequency fundamentals for H₂-tagged protonated glycine

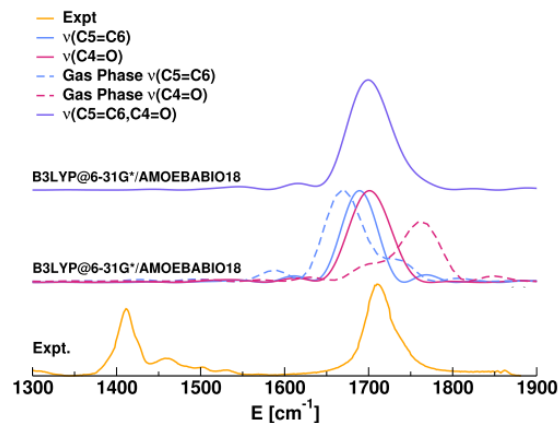


- Quantum interference effects between states just below and just above the rotational barrier of the NH₃.
More on comparisons between semiclassical and classical calculations in **R.Conte et al. *Theor. Chem. Acc.* **142**, 53 (2023).**

SC spectroscopy of solvated species

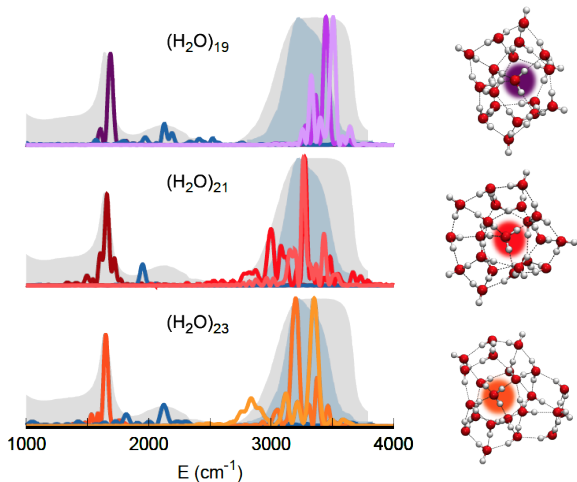


Thymidine
in water



DC SCIVR calculations at QM/MM level are able to reproduce experimental degeneracy of C=O and C=C stretches of thymidine solvated by water.

D. Moscato, G. Mandelli, M. Bondanza, F. Lipparini, **R. Conte**, B. Mennucci, M. Ceotto *J. Am. Chem. Soc.* **146**, 8179 (2024).



Study of water cluster solvation employing a many-body PIP PES.

The central water molecule is spectroscopically solvated when surrounded by 20 water molecules

A. Rognoni, **R. Conte**, M. Ceotto *Chem. Sci.* **12**, 2060 (2021).

Time-averaged semiclassical IR spectra

- SC IR spectra can be calculated starting from power spectra and by means of a state-to-state IR expression, but need calculation of SC eigenfunctions or decomposition of the IR spectrum in terms of several SC power spectra

M. Micciarelli, J. Suarez, **R. Conte**, M. Ceotto *J. Chem. Phys.* **149**, 064115 (2018).

M. Micciarelli, F. Gabas, **R. Conte**, M. Ceotto *J. Chem. Phys.* **150**, 184113 (2019).

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- It is possible to work out a time averaged formula also for absorption spectra

$$\alpha(\omega, T) = \omega(1 - e^{-\beta\hbar\omega})\sigma(\omega, T) \quad \text{IR SPECTRUM (relative intensities)}$$

$$\sigma(\omega, T) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} dt e^{-i\omega t} C_{\mu\mu}(t, T) \quad \text{Absorption lineshape}$$

$$C_{\mu\mu}(t, T) = \langle \hat{\mu}(0)\hat{\mu}(t) \rangle = \text{Tr} \left[\hat{B}(\beta) \hat{\mu} e^{i\hat{H}t/\hbar} \hat{\mu} e^{-i\hat{H}t/\hbar} \right]$$

$\hat{B}(\beta)$ is the Boltzmann operator and $\beta = 1/k_B T$

Time-averaged semiclassical IR spectra

$$C_{\mu\mu}(t, T) = \langle \hat{\mu}(0)\hat{\mu}(t) \rangle = \text{Tr} \left[\hat{B}(\beta) \hat{\mu} e^{i\hat{H}t/\hbar} \hat{\mu} e^{-i\hat{H}t/\hbar} \right]$$

Splitting of Boltzmann operator

Cyclic permutation rule



$$C_{\mu\mu}(t, T) = \text{Tr} \left[\hat{B}(\beta/2) \hat{\mu} e^{i\hat{H}t/\hbar} \hat{\mu} \hat{B}(\beta/2) e^{-i\hat{H}t/\hbar} \right]$$

Herman-Kluk propagator

Time average



$$\sigma(\omega, T) = \frac{(2\pi\hbar)^{-2N_\nu}}{2\pi T_s} \iint d\mathbf{p}_0 d\mathbf{Q}_0 \iint d\mathbf{p}'_0 d\mathbf{Q}'_0$$

$$\times \left| \int_0^{T_s} dt e^{i[S_t(\mathbf{p}'_0, \mathbf{Q}'_0) - S_t(\mathbf{p}_0, \mathbf{Q}_0) - \hbar\omega t + \phi'(t) - \phi(t)]/\hbar} \langle \mathbf{p}_t \mathbf{Q}_t | \hat{\mu} \hat{B}(\beta/2) | \mathbf{p}'_t \mathbf{Q}'_t \rangle \right|^2$$

Time-averaged semiclassical IR spectra

$$\sigma(\omega, T) = \frac{(2\pi\hbar)^{-2N_\nu}}{2\pi T_s} \iint d\mathbf{p}_0 d\mathbf{Q}_0 \iint d\mathbf{p}'_0 d\mathbf{Q}'_0 \times \left| \int_0^{T_s} dt e^{i[S_t(\mathbf{p}'_0, \mathbf{Q}'_0) - S_t(\mathbf{p}_0, \mathbf{Q}_0) - \hbar\omega t + \phi'(t) - \phi(t)]/\hbar} \langle \mathbf{p}_t \mathbf{Q}_t | \hat{\mu} \hat{B}(\beta/2) | \mathbf{p}'_t \mathbf{Q}'_t \rangle \right|^2$$

- Low temperature limit ($T \rightarrow 0$ $\beta \rightarrow +\infty$)

$$\hat{B}(\beta) = \frac{e^{-\beta\hat{H}}}{Z} \quad Z \approx e^{-\beta E_0} \quad \hat{B}(\beta) \approx |\Psi_0\rangle\langle\Psi_0|$$

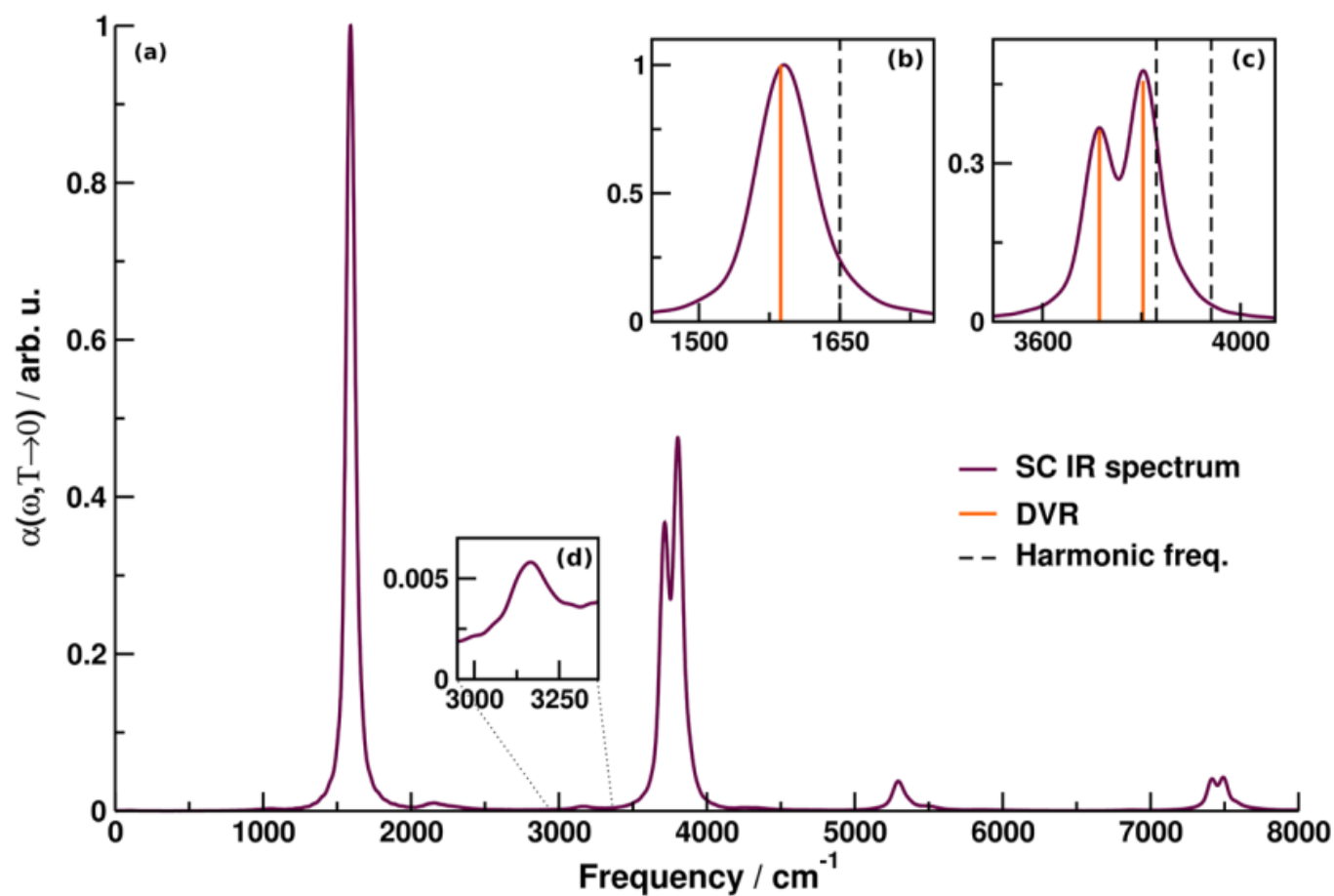
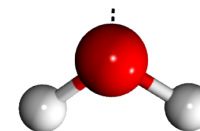
$$\langle \mathbf{p}_t \mathbf{Q}_t | \hat{\mu} \hat{B}(\beta/2) | \mathbf{p}'_t \mathbf{Q}'_t \rangle = \langle \mathbf{p}_t \mathbf{Q}_t | \hat{\mu} | \Psi_0 \rangle \langle \Psi_0 | \mathbf{p}'_t \mathbf{Q}'_t \rangle$$

- $|\Psi_0\rangle$ is approximated to the ground state of a harmonic oscillator

- Dipole is linearized $\mu(\mathbf{q}) - \mu(\mathbf{q}_{eq}) \simeq \sum_{j=1}^{N_\nu} \left. \frac{\partial \mu}{\partial q_j} \right|_{\mathbf{q}_{eq}} (q_j - q_{eq,j})$

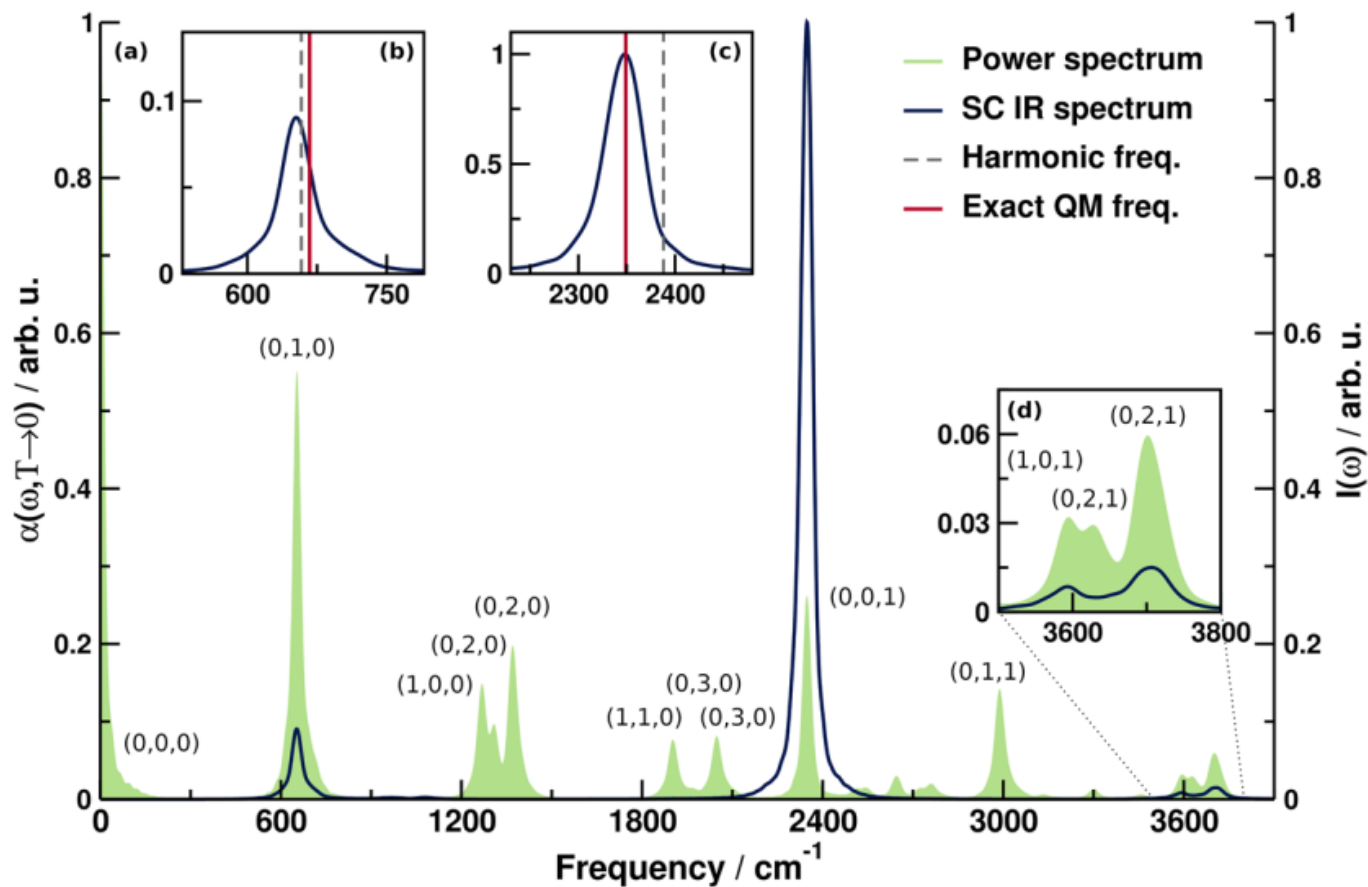
Time-averaged semiclassical IR spectra

- SC IR spectrum of the water molecule



Time-averaged semiclassical IR spectra

- Comparison between SC power spectrum and SC IR spectrum of CO_2



Summary and Perspectives

- PIP PESs are highly accurate and fast to evaluate. Developed up to ~ 40 atoms



Improving quality of PIP fitting basis set to
Build PIP PESs for larger and larger systems

- SC vibrational spectroscopy is accurate and able to deal with large systems



Interface time-averaged SC IR spectroscopy with techniques developed for
power spectra and perform calculations at finite temperature

Thank you for your attention!