TENSOR TRAINS FOR HIGHLY MULTIDIMENSIONAL DYNAMICS SIMULATIONS

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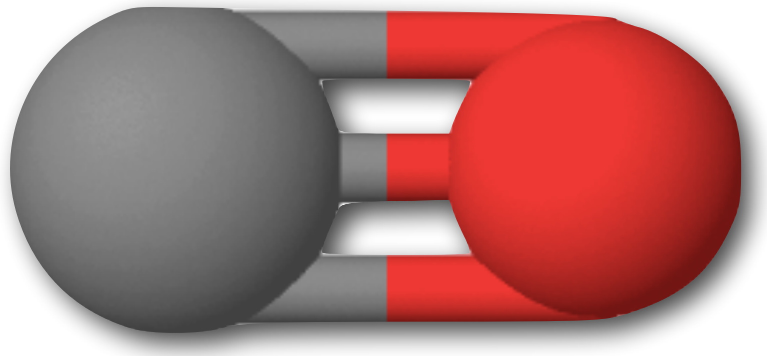
VIRTUAL INTERNATIONAL SEMINAR ON THEORETICAL ADVANCEMENTS (VISTA)

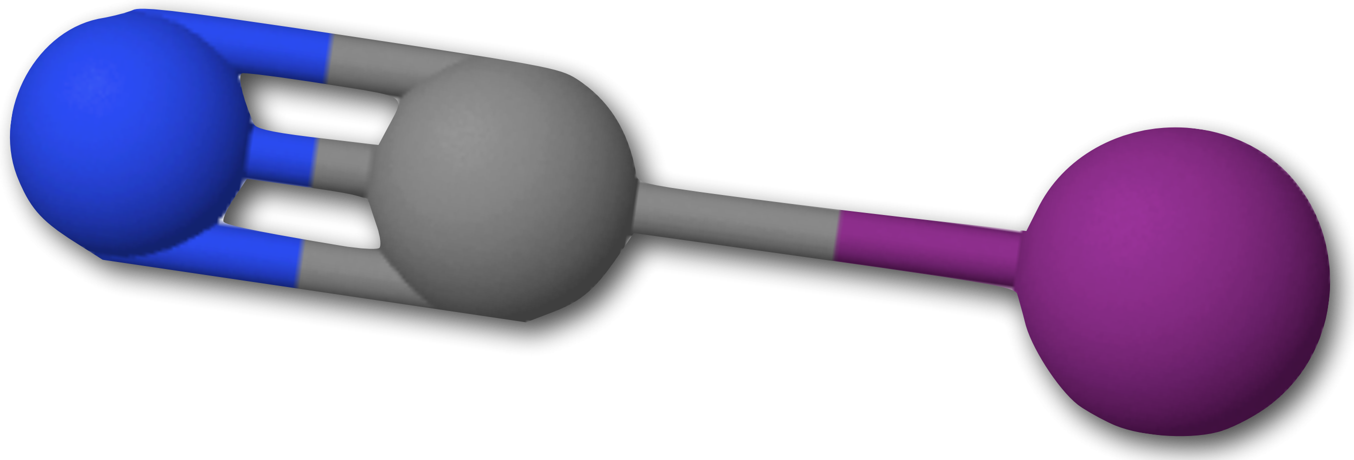
Image reproduced from J. Olson, et al, 2016, arXiv:1706.05413

CURSE OF DIMENSIONALITY

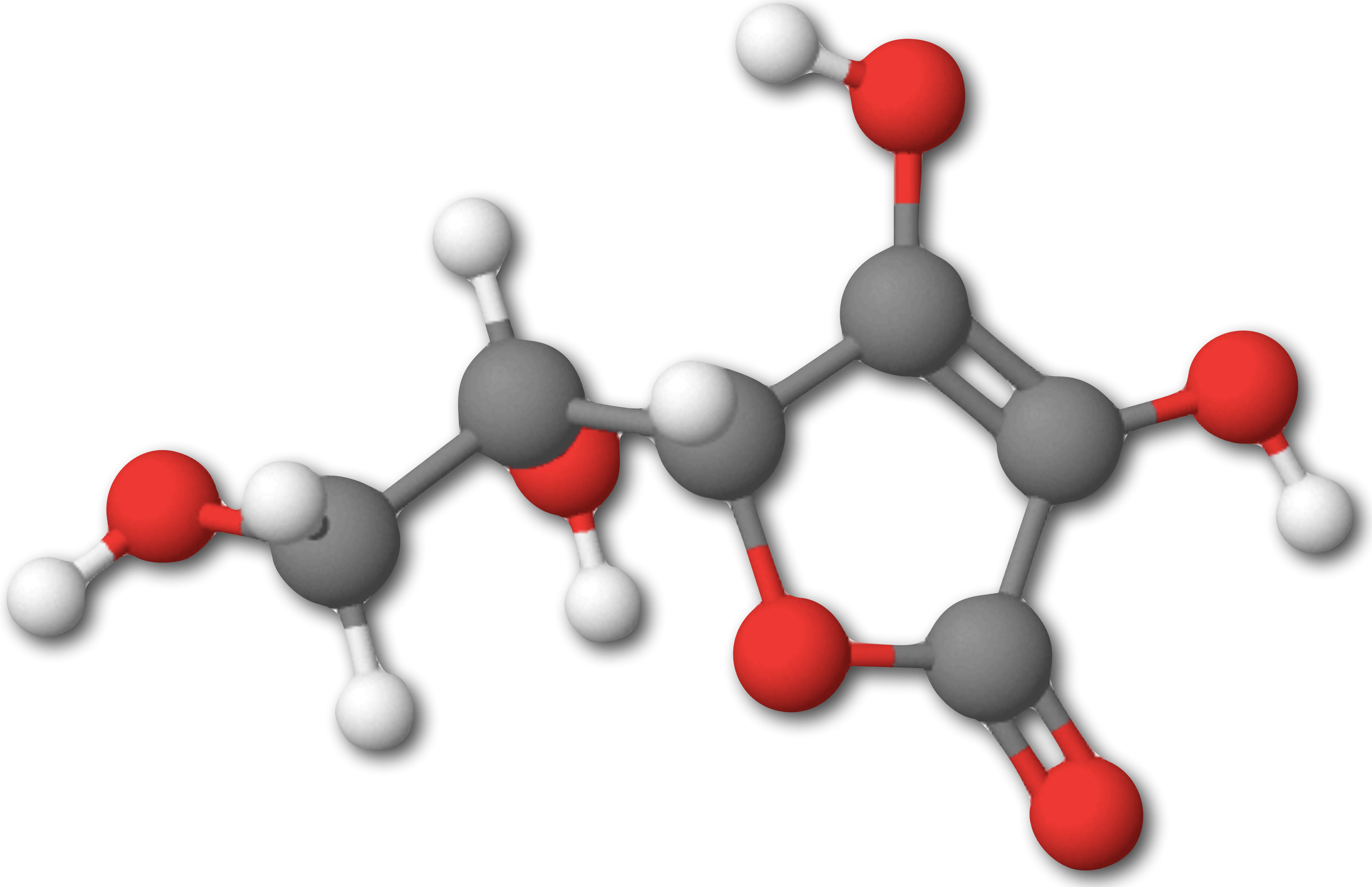
Many classical computer approaches to quantum mechanics simulations become computationally intractable for large molecular systems.



2 Atoms:
2 KB



3 Atoms:
100 MB



20 Atoms:
10^{119} TB

LOW-RANK TENSOR-TRAIN DECOMPOSITION REDUCES COST

Original Image

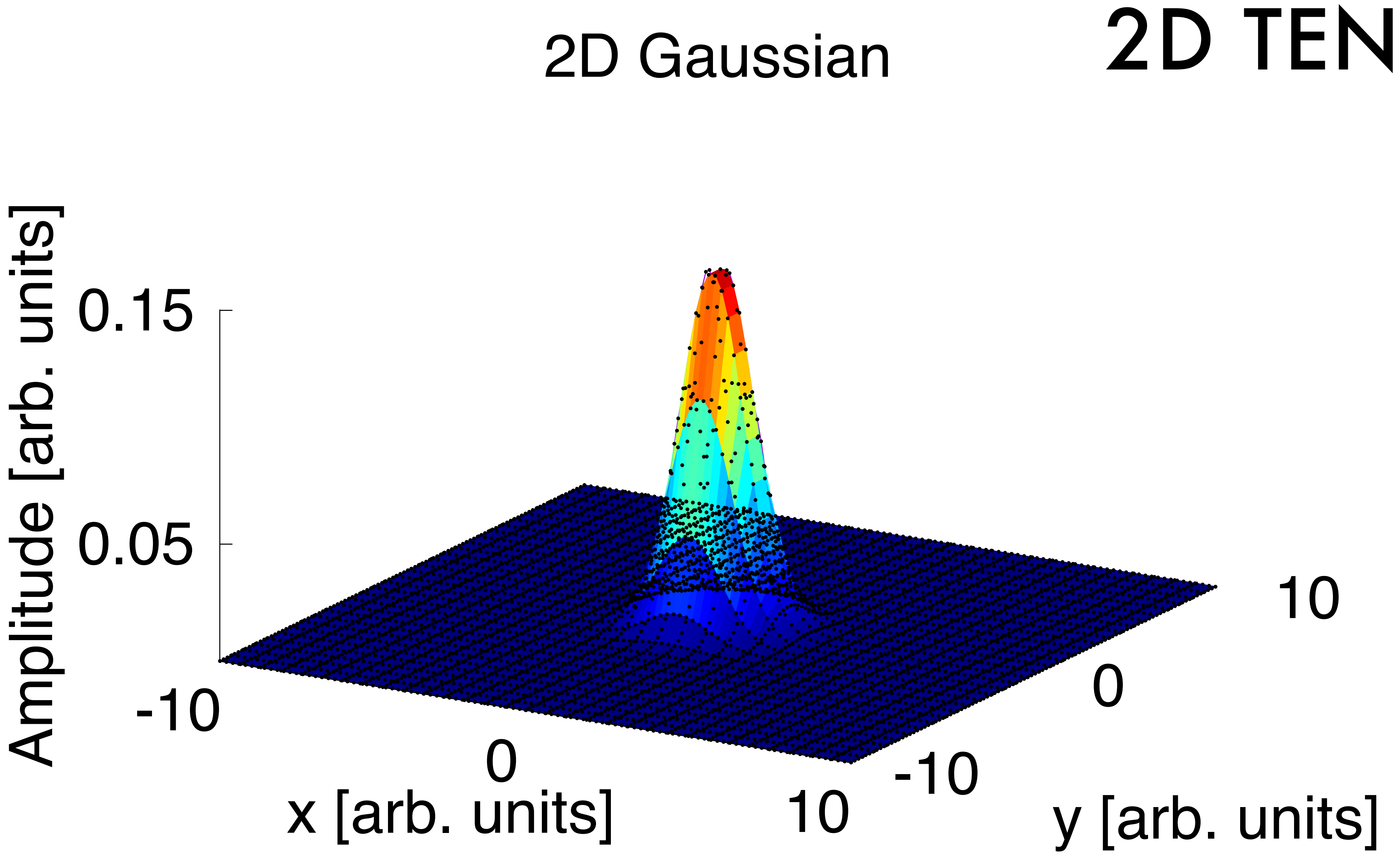
100%

Tensor Train

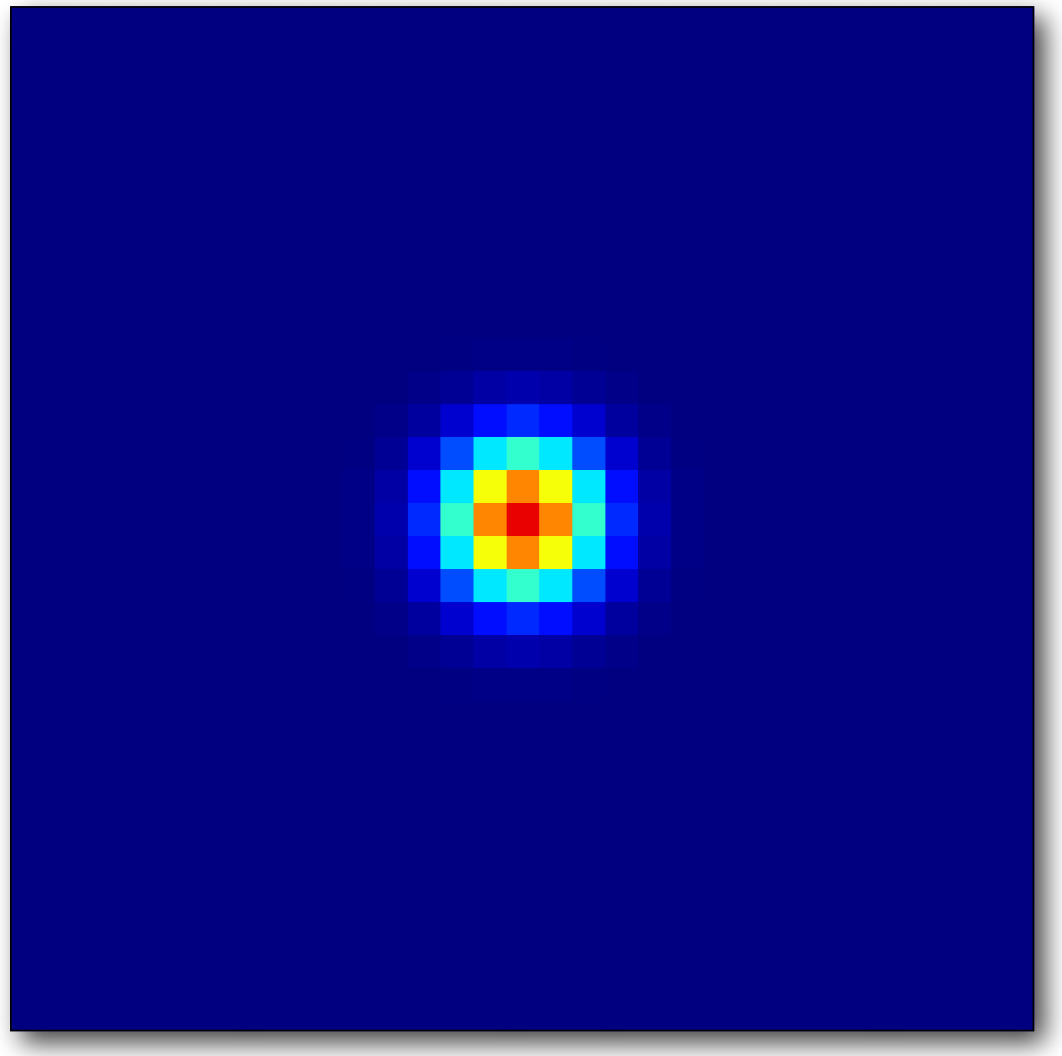
15%

N. Lyu*, E. Mulvihill*, **Micheline B. Soley**, E. Geva, V. S. Batista, (2023) JCTC, in press.
T. H. Kyaw*, **Micheline B. Soley**,* B. Allen, P. Bergold, C. Sun, V. S. Batista, A. Aspuru-Guzik, (2022) arXiv:2208.10470v1.
Micheline B. Soley,* P. E. Videla,* E. T. J. Nibbering, V. S. Batista, J. Phys. Chem. Lett., 13 (2022) 8354.
Micheline B. Soley, P. Bergold, A. A. Gorodetsky, V. S. Batista, JCTC, 18 (2022) 25.
Y. Wang, E. Mulvihill, Z. Hu, N. Lyu, S. Shivpuje, Y. Liu, **Micheline B. Soley**, E. Geva, V. S. Batista, S. Kais, 2022, arXiv:2209.04956.
N. Lyu, **Micheline B. Soley**, V. S. Batista, JCTC, 18 (2022) 3327.
Micheline B. Soley, P. Bergold, V. S. Batista, JCTC 17 (2021) 3280.
B. N. Khoromskij, Constr. Approx. 34 (2011) 257.
I. Oseledets, E. Tyryshnikov, Linear Algebra Appl. 432 (2010) 70.
J. C. Napp, et al. Phys. Rev. X 12 (2022) 021021.

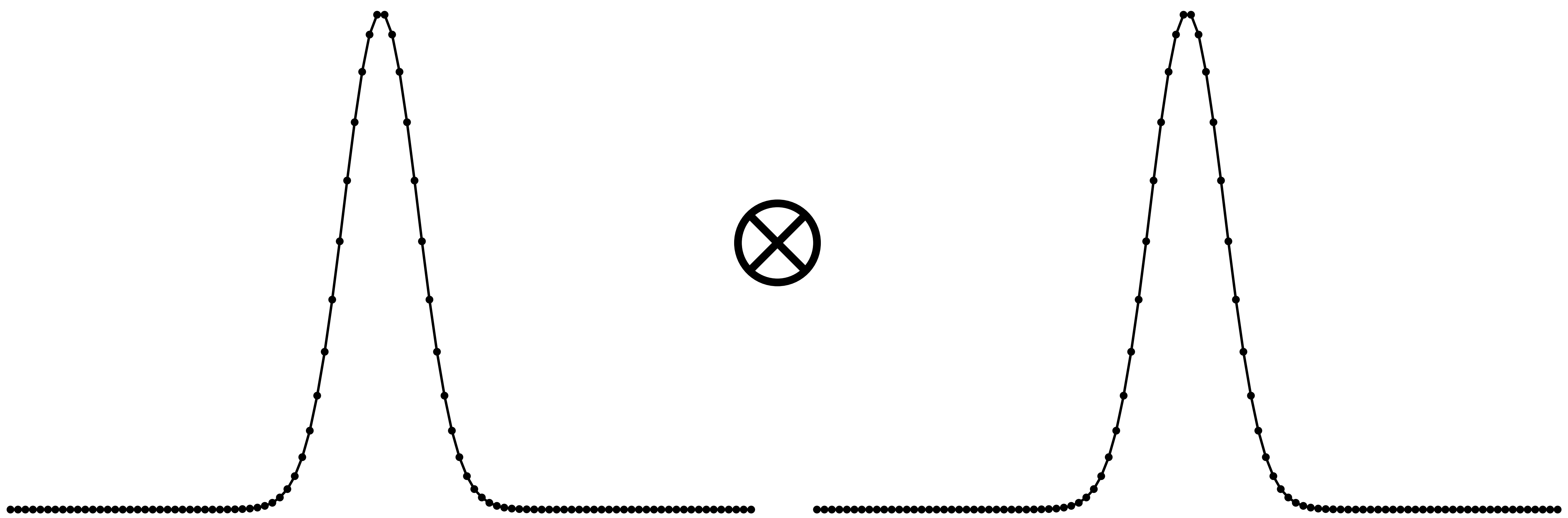
2D TENSOR TRAIN (RANK 1)



$$\Psi(x,y) = \frac{1}{2\pi}\exp\left(-\frac{x^2}{2} - \frac{y^2}{2}\right)$$

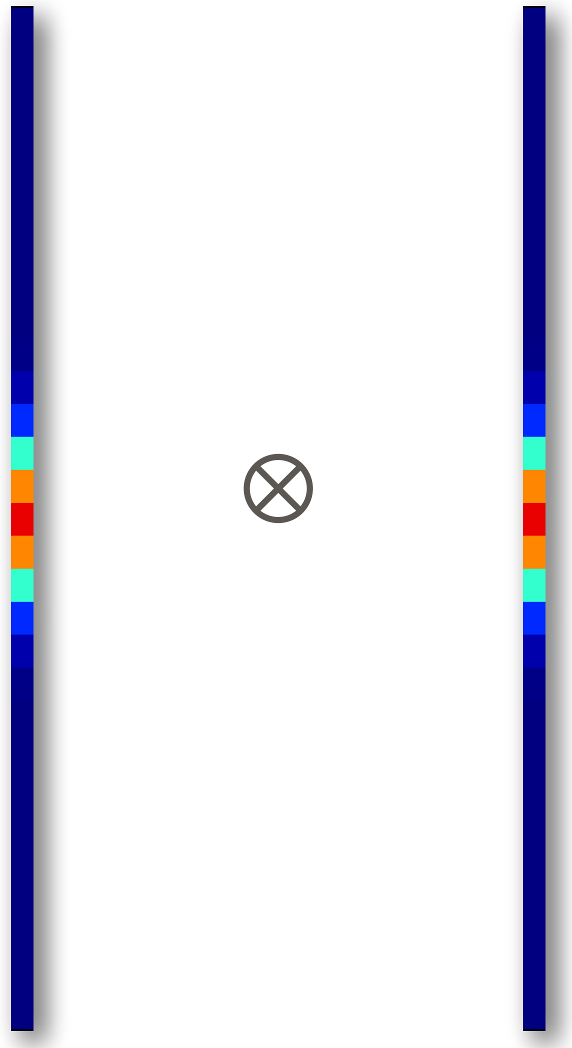


vs.



$$\psi(x)\psi(y) = \left(\frac{1}{\sqrt{2\pi}}\exp\left(-\frac{x^2}{2}\right)\right)\left(\frac{1}{\sqrt{2\pi}}\exp\left(-\frac{y^2}{2}\right)\right)$$

$$= \sum_{\alpha=1}^{r} \psi_1(1,x,\alpha)\psi_2(\alpha,y,1)$$

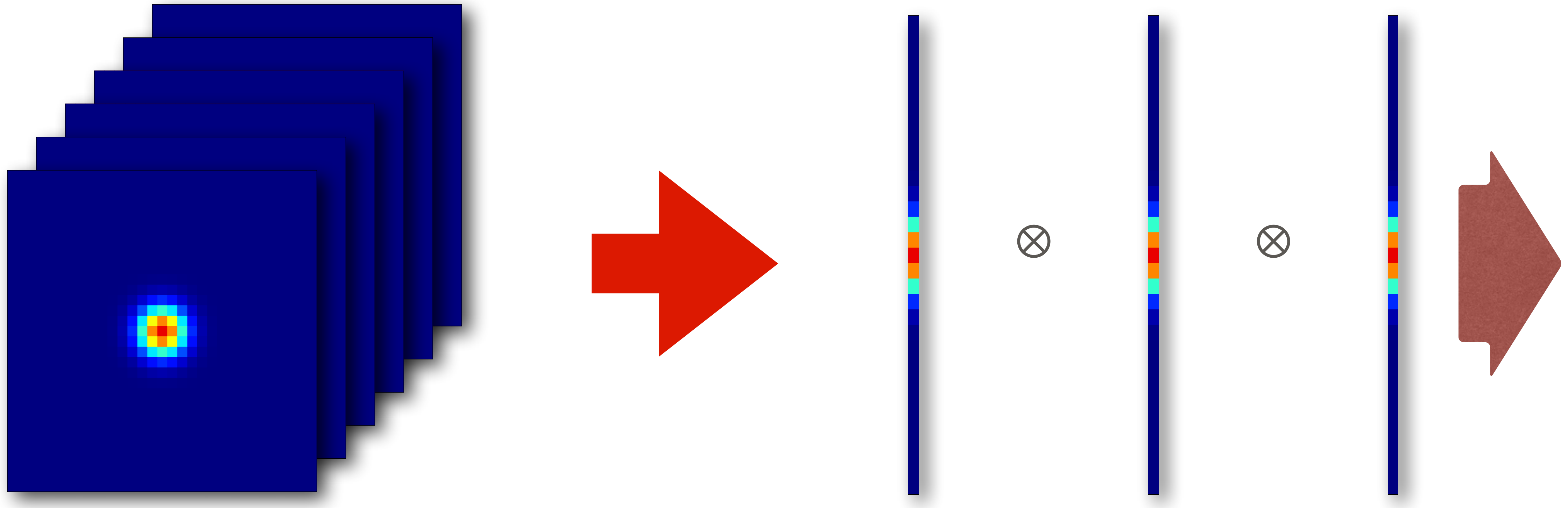


Cost of evaluating reduces to

$$n^2 \rightarrow 2n$$

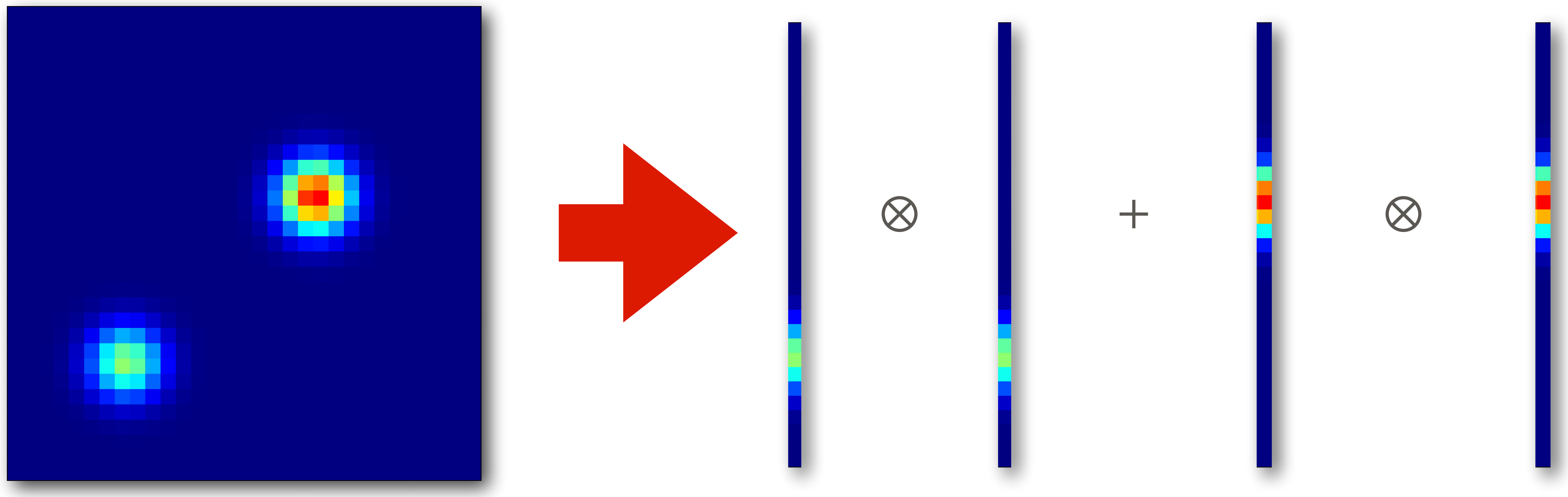
I. V. Oseledets, *SIAM J. Sci Comput.* 33 (2011) 2295

ND TENSOR TRAIN (RANK 1)



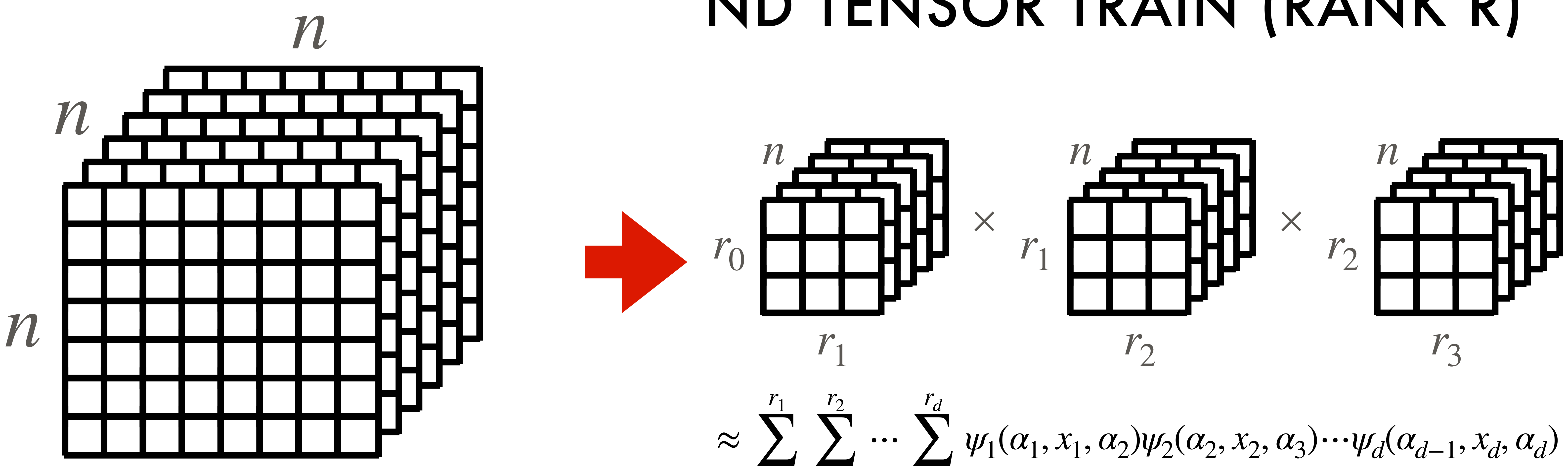
Cost Reduction: $n^3 \to 3n$

2D TENSOR TRAIN (RANK 2)



Cost Reduction: $n^2 \to 2 \times 2n$

ND TENSOR TRAIN (RANK R)



$\Psi(x_1, x_2, \cdots, x_d)$

$$\approx \sum_{\alpha_1=1}^{r_1} \sum_{\alpha_2=1}^{r_2} \cdots \sum_{\alpha_d=1}^{r_d} \psi_1(\alpha_1, x_1, \alpha_2)\psi_2(\alpha_2, x_2, \alpha_3)\cdots\psi_d(\alpha_{d-1}, x_d, \alpha_d)$$

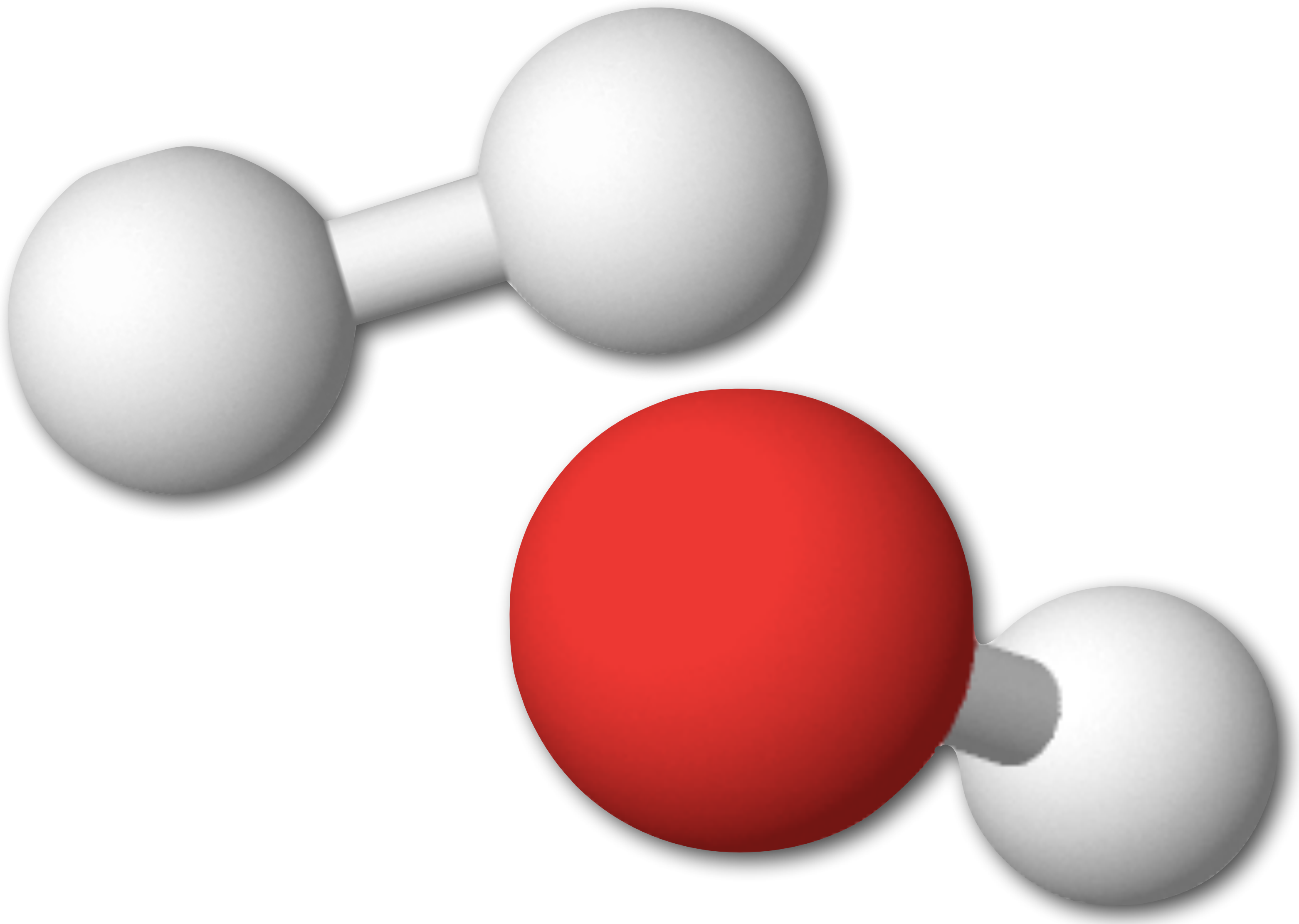
Cost Reduction

$n^d \to dnr^2$

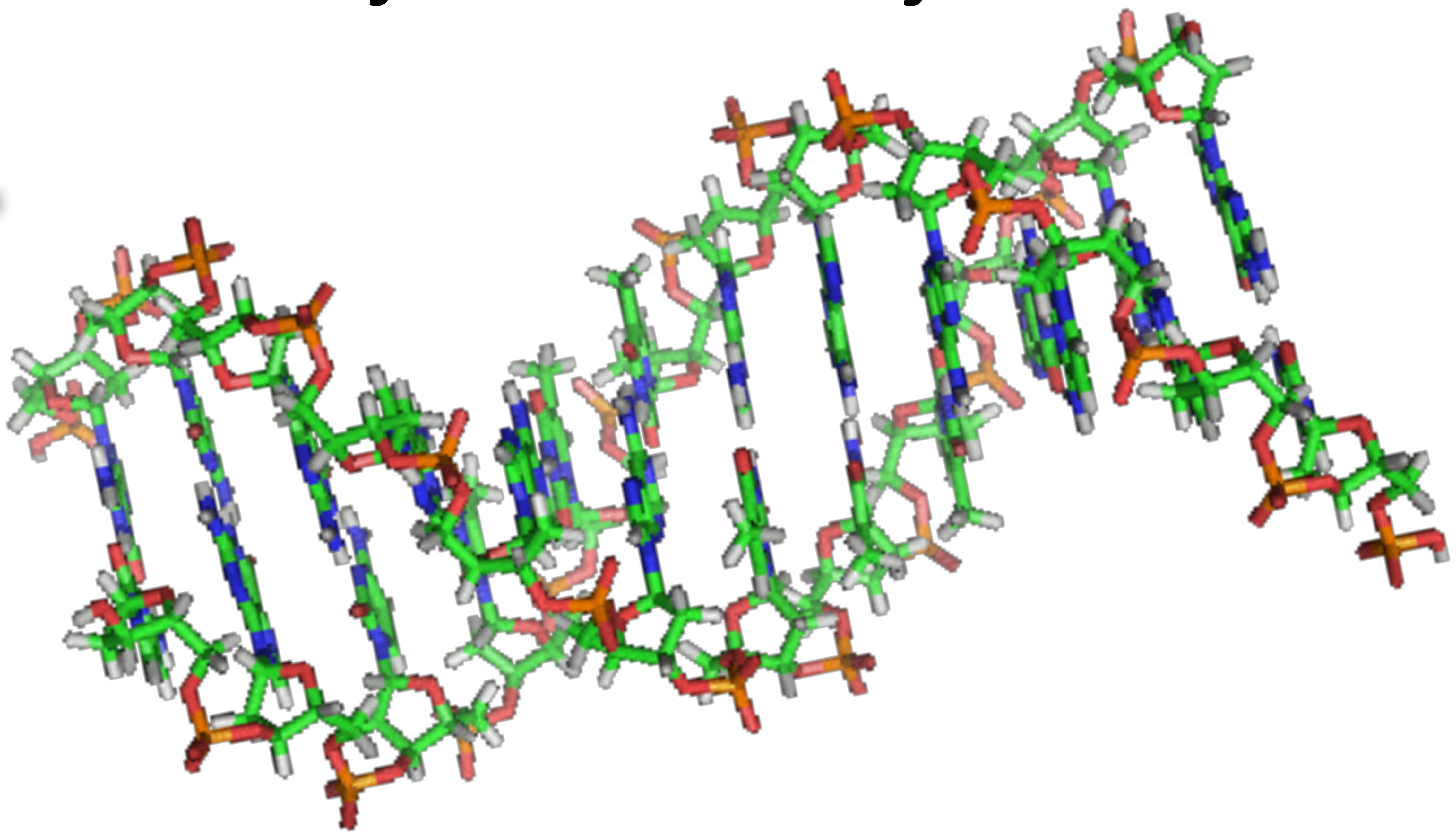
M.-L. Li, K. S. Candan, M. L. Salino, "GTT: Guiding the tensor train decomposition." International Conference on Similarity Search and Applications. Springer, Cham, 2020.
I. Oseledets, E. Tyryshnikov, Linear Algebra Appl. 432 (2010) 70.

TENSOR TRAINS FOR HIGHLY MULTIDIMENSIONAL QUANTUM DYNAMICS

Largest System Investigable with Standard Chebyshev Dynamics



Functional Tensor-Train Chebyshev (FTTC) Dynamics

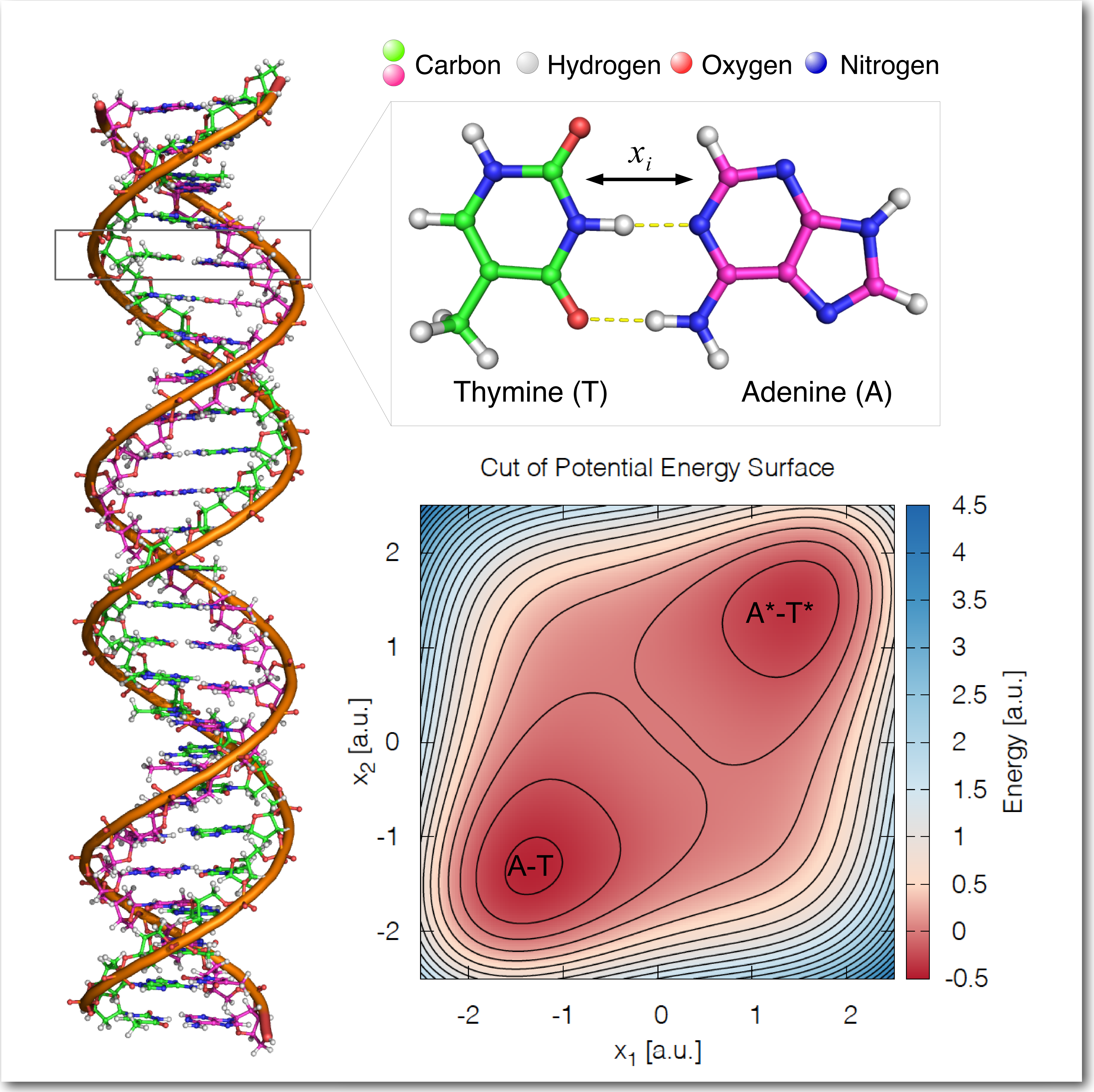


M. T. Cvitaš, S. C. Althorpe, J. Chem. Phys. 139 (2013) 064307.
E. M. Goldfield, S. K. Gray, J. Chem. Phys. 117 (2002) 1604.
H. Tal-Ezer, R. Kosloff, J. Chem. Phys. 81 (1984) 3967.

Micheline B. Soley, P. Bergold, A. A. Gorodetsky, V. S. Batista, JCTC, 18 (2022) 25.

FUNCTIONAL TENSOR TRAIN CHEBYSHEV (FTTC) DYNAMICS

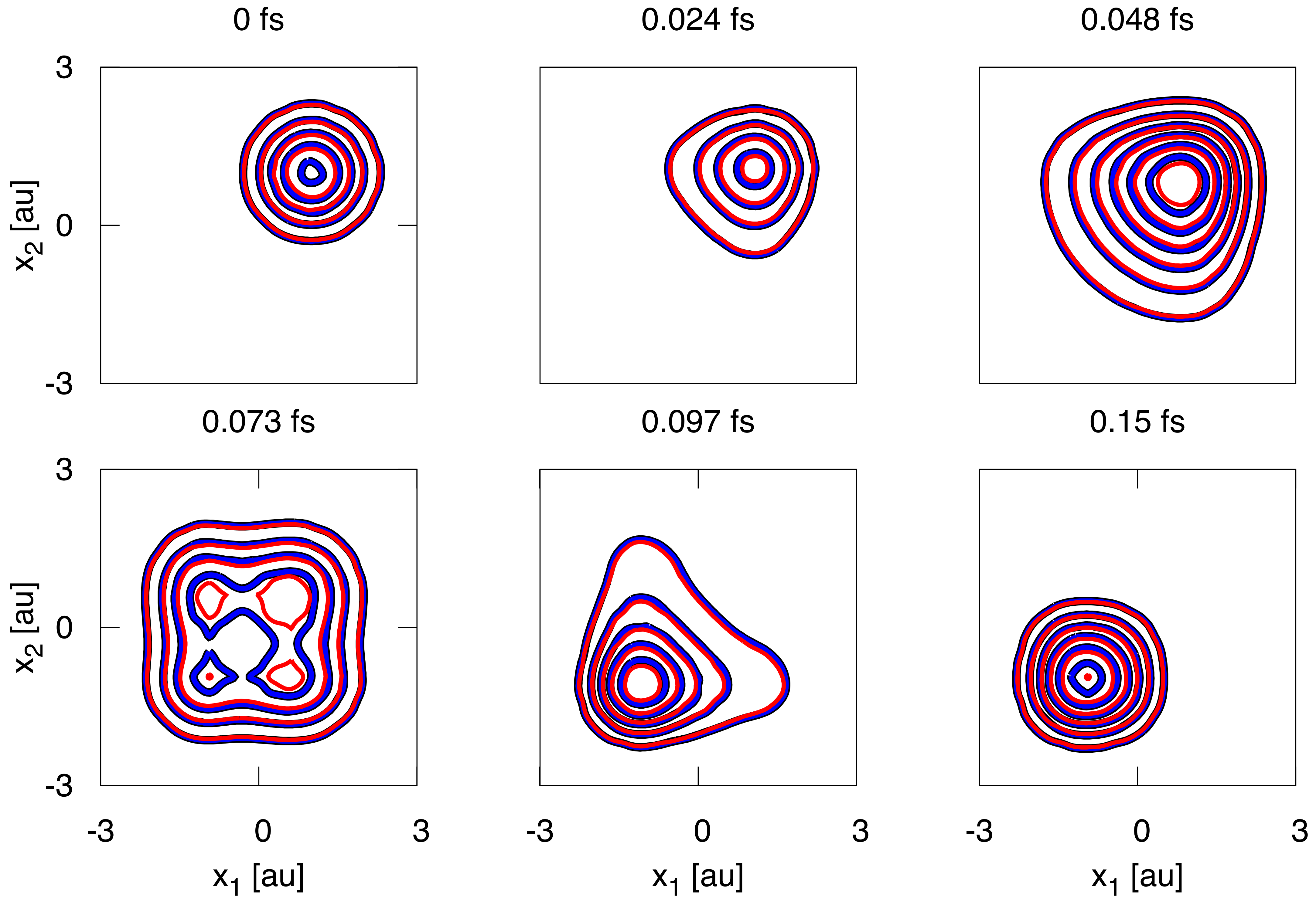
$$\Psi(t) = e^{-it\hat{H}}\Psi(0)$$
$$\approx e^{-it^{+}} \sum_{k=0}^{N-1} (2-\delta_{k,0})(-i)^k J_k(t^{-}) T_k(\hat{\mathbf{H}}_0)\mathbf{W}_0$$



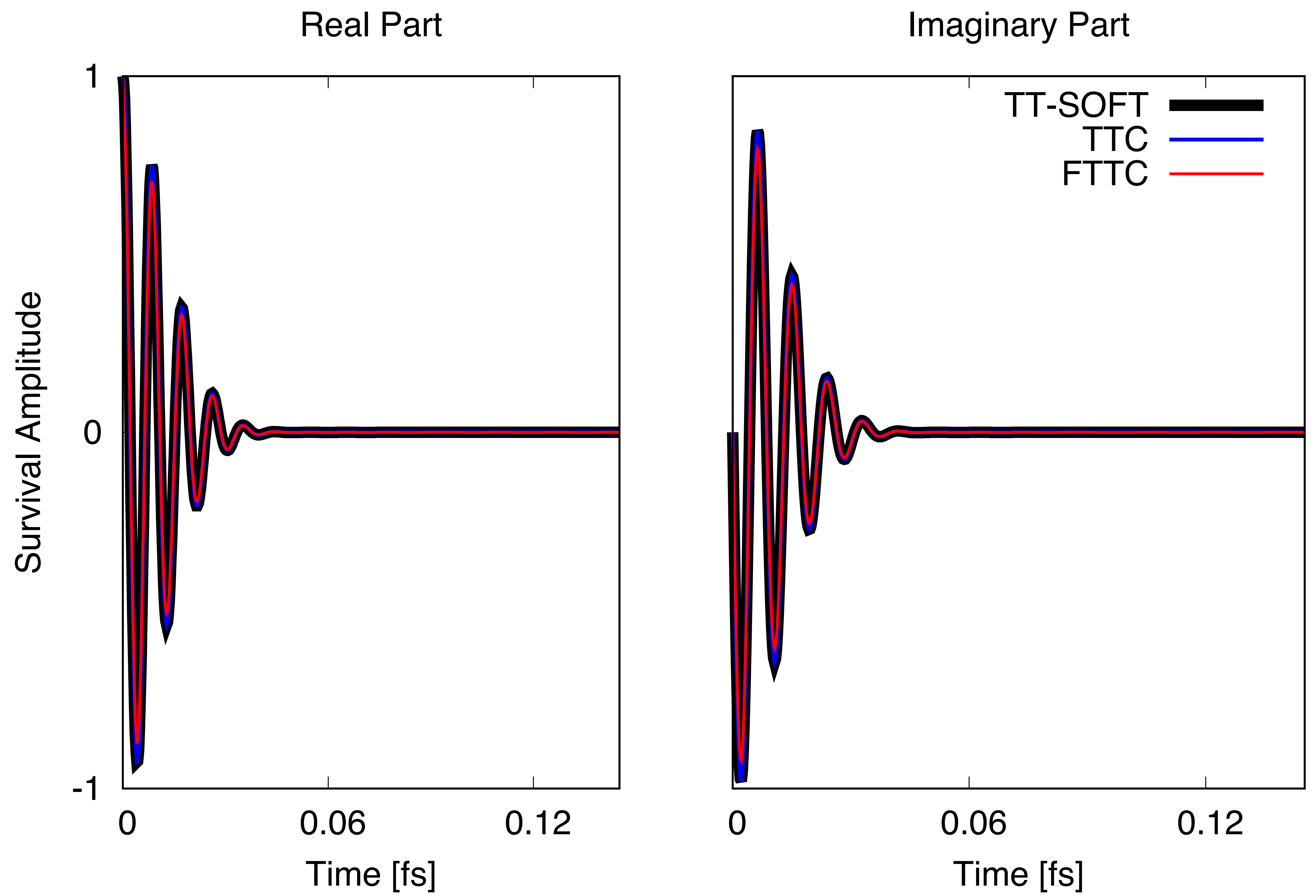
Micheline B. Soley, P. Bergold, A. A. Gorodetsky, V. S. Batista, JCTC, 18 (2022) 25.

APPLICATION: HYDROGEN BONDING IN DNA

Probability Density Dynamics, Uncoupled Bath



Survival Amplitude



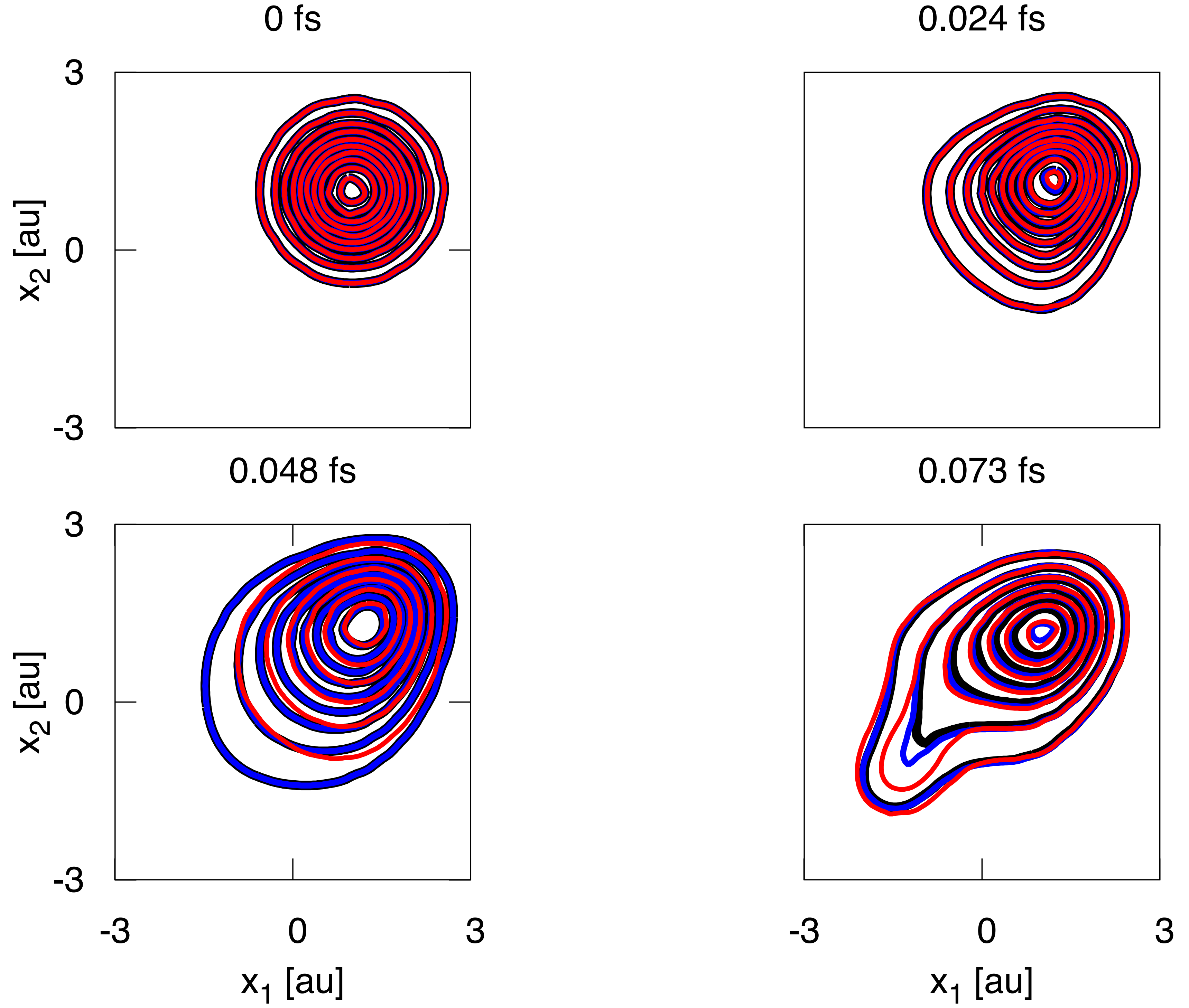
FTTC extends the Chebyshev method from simulation of four-atom systems to molecular systems in

50 dimensions.

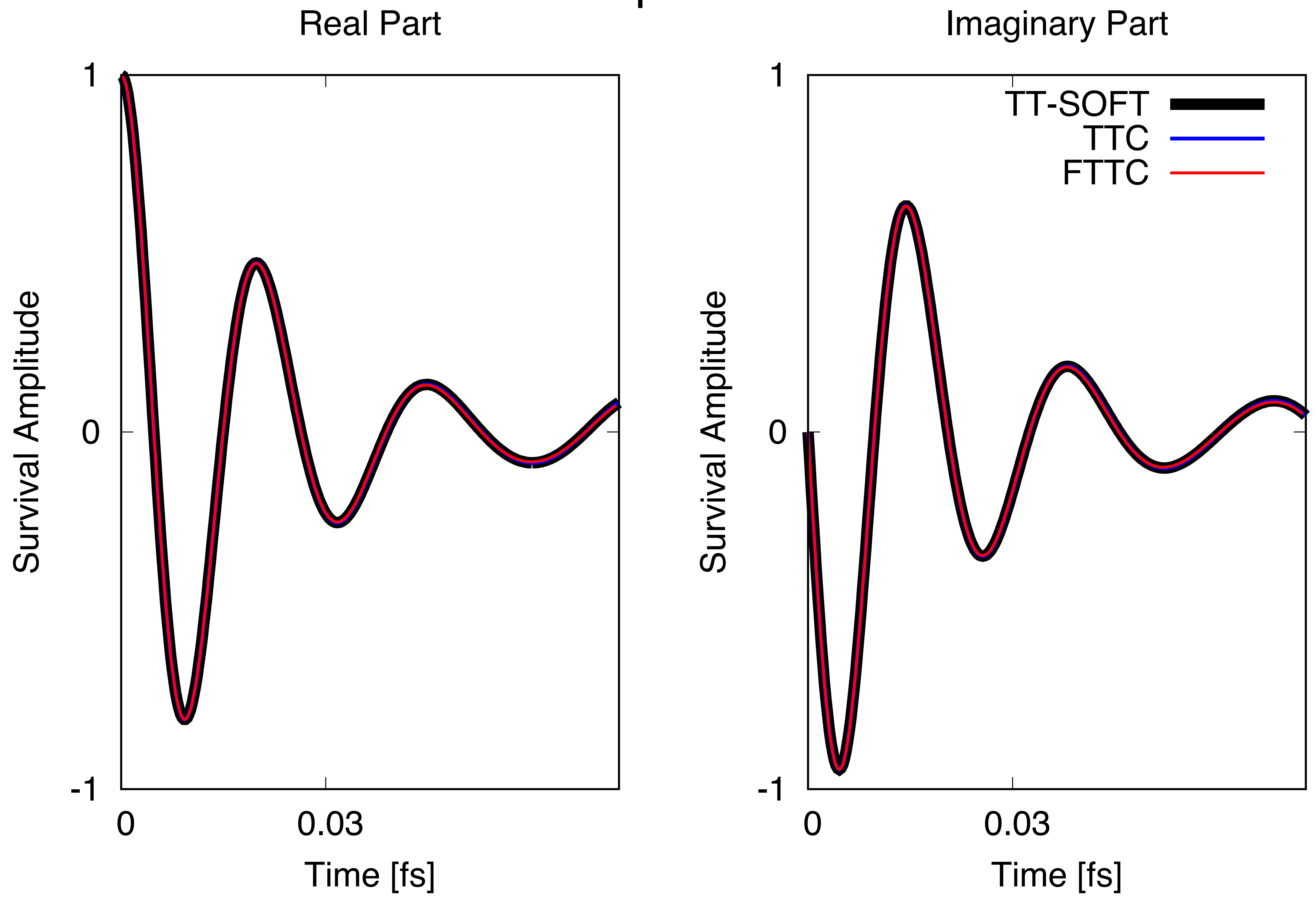
Micheline B. Soley, P. Bergold, A. A. Gorodetsky, V. S. Batista, JCTC, 18 (2022) 25.

COUPLED HYDROGEN BONDING IN DNA

Probability Density Dynamics, Anharmonically Coupled Bath



Survival Amplitude



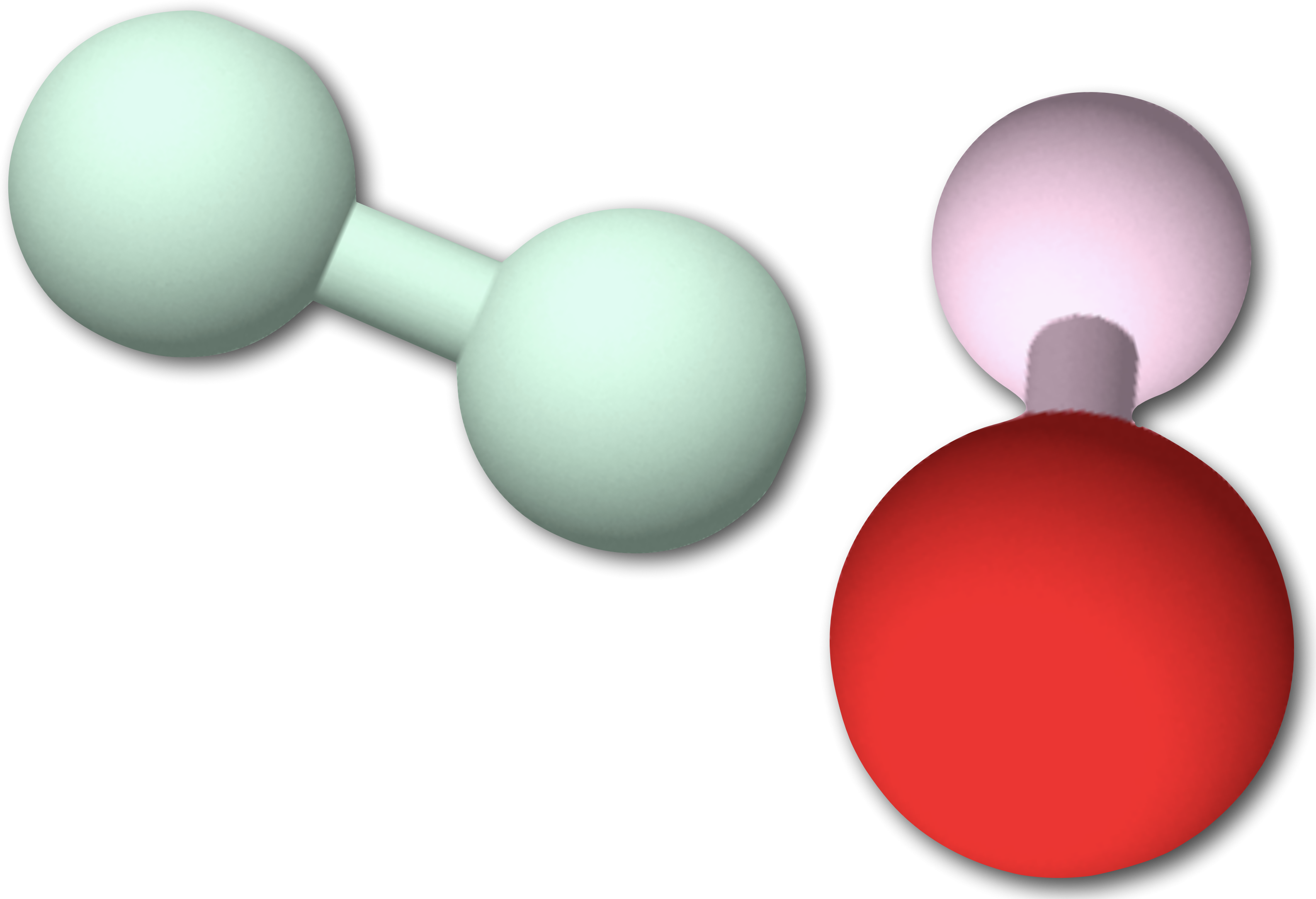
FTTC successfully determines molecular dynamics

even with significant coupling of atomic motion between modes.

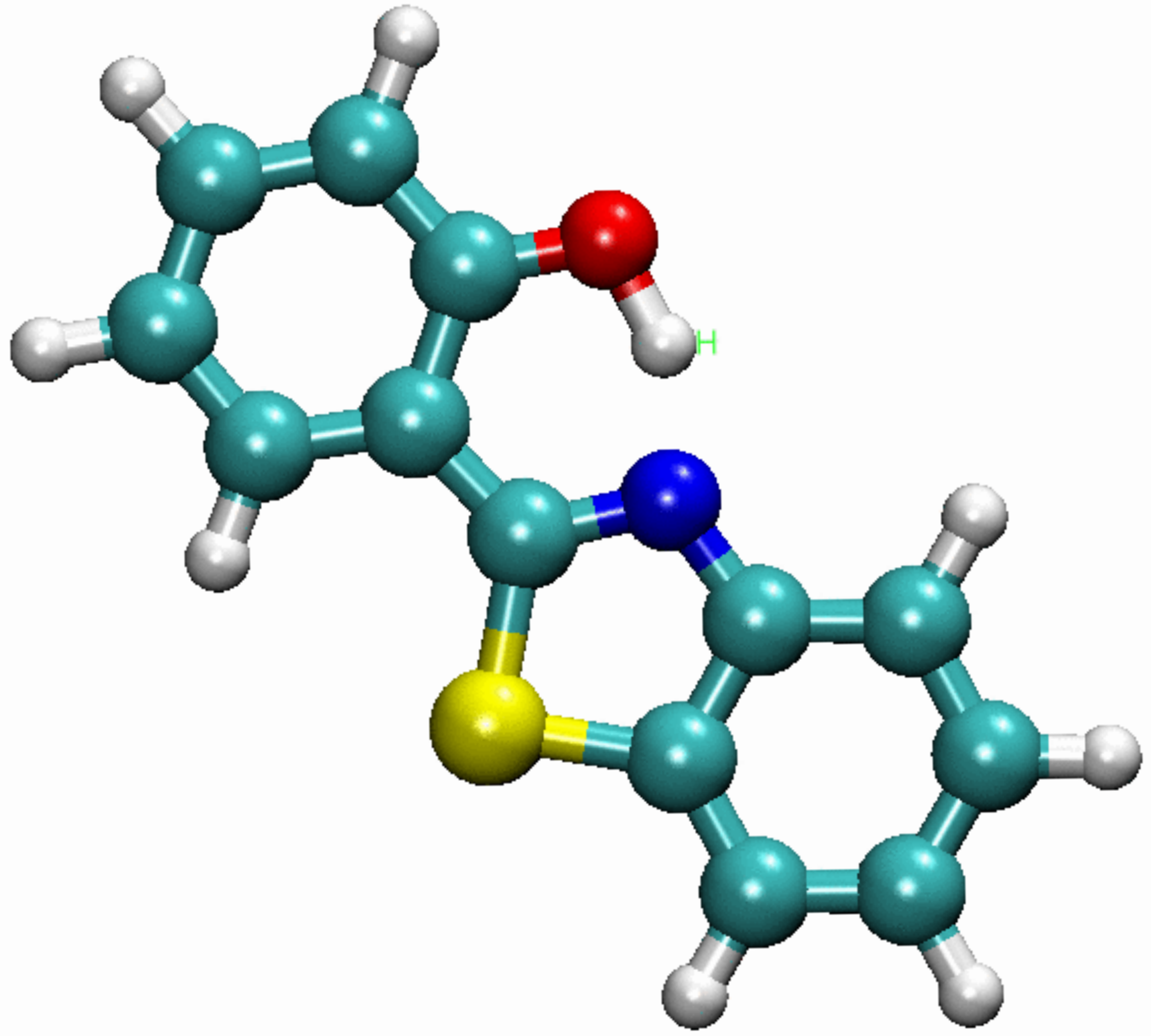
Micheline B. Soley, P. Bergold, A. A. Gorodetsky, V. S. Batista, JCTC, 18 (2022) 25.

TENSOR-TRAINS FOR UV-PUMP/X-RAY PROBE SPECTROSCOPY

Largest System Investigable with Standard Fixed-Grid SOFT Dynamics



Tensor-Train Split-Operator Fourier Transform (TT-SOFT) Dynamics

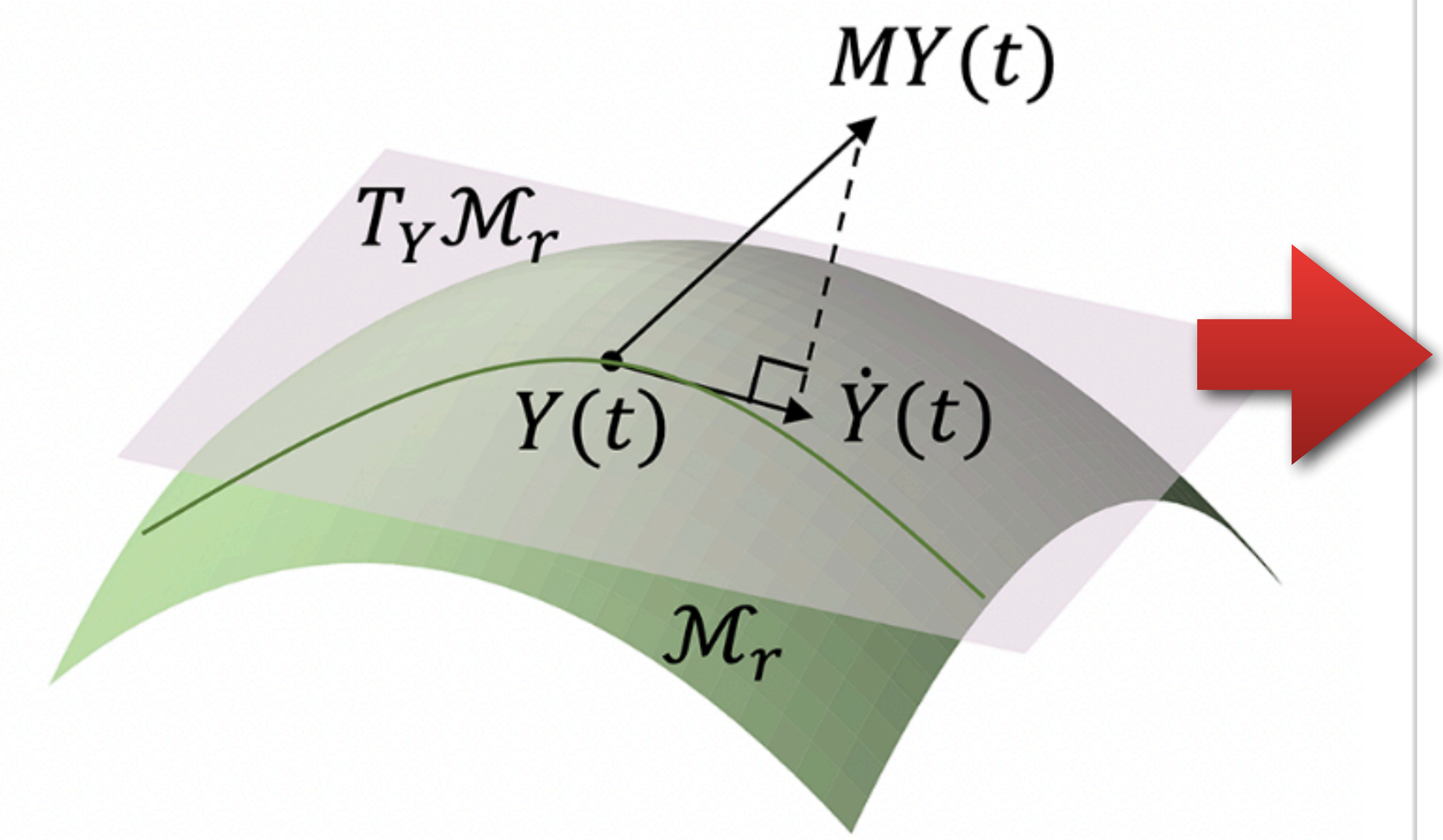


J. A. Fleck Jr., A. Steiger, J. Comput. Phys. 47 (1982) 412.
S. M. Greene, V. S. Batista, JCTC 13 (2017) 4034.

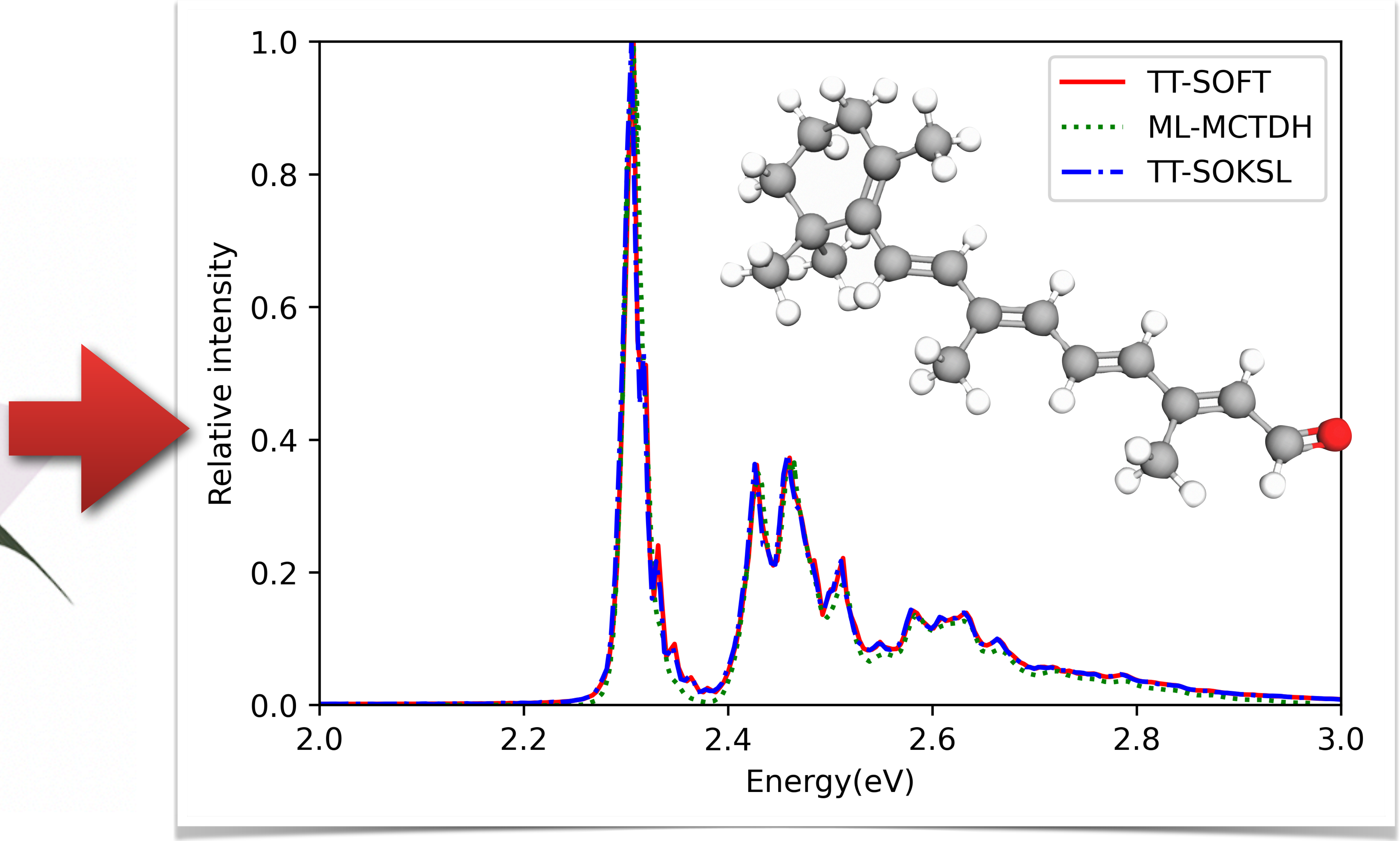
Micheline B. Soley,* P. E. Videla,* E. T. J. Nibbering, V. S. Batista, (2022) J. Phys. Chem. Lett., 18 (2022) 8254.

NOVEL TENSOR-TRAIN MOLECULAR METHODS

TT-KSL



Tensor-Train Split-Operator KSL (TT-SOKSL) Dynamics



Micheline B. Soley, N. Lyu, V. S. Batista, JCTC, 18 (2022) 3327.

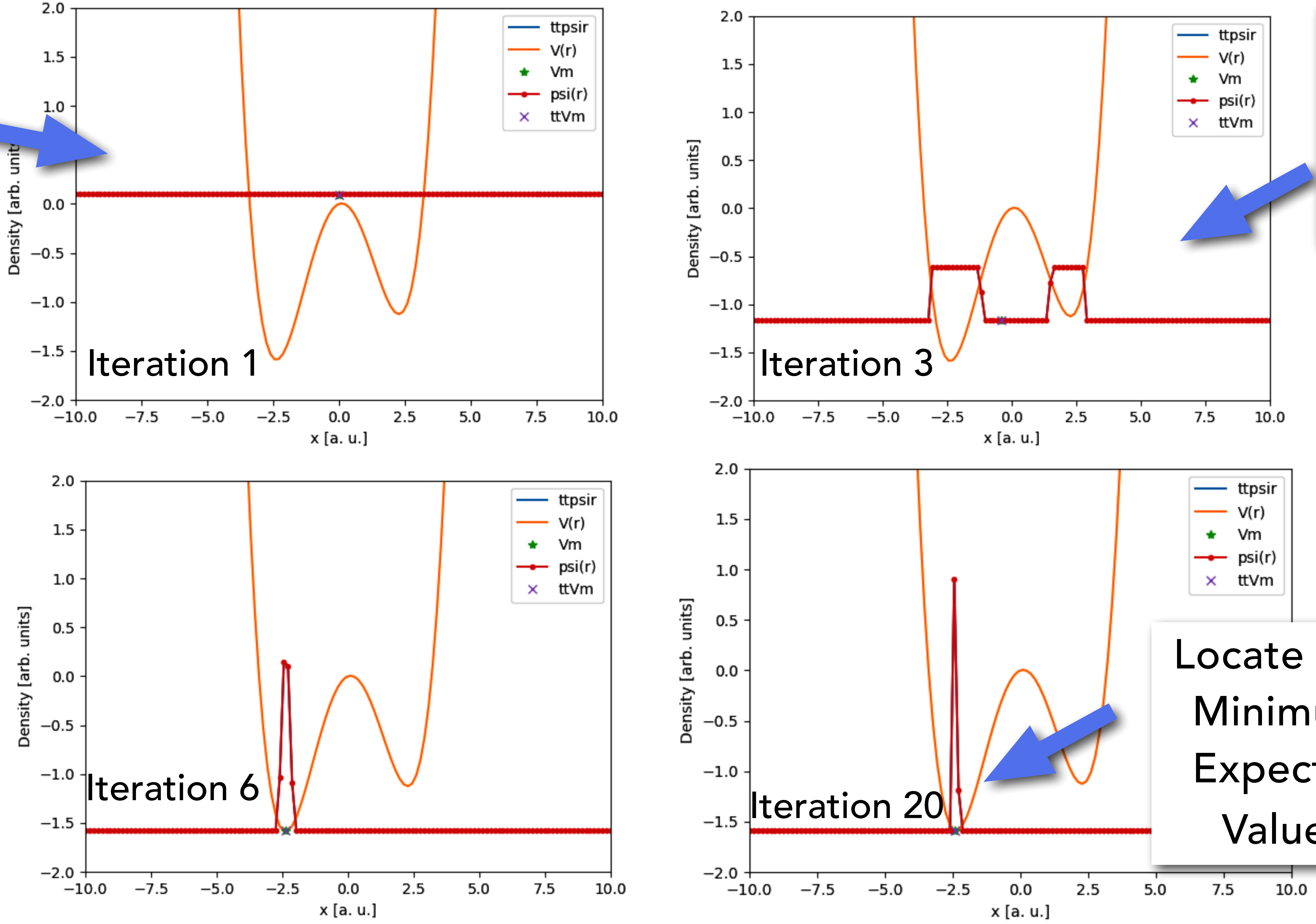
C. Lubich, From Quantum to Classical Molecular Dynamics: Reduced Models and Numerical Analysis, European Mathematical Society, 2009.

TENSOR-TRAIN ITERATIVE POWER ALGORITHM (IPA)

Initialize ρ and V as Tensor Trains

Iteratively Apply Oracle

$$\rho(x) \to \mathcal{N}U(x)\rho(x)$$
$$U(x) = e^{-cV(x)}$$



Locate Global Minimum as Expectation Value $\langle x \rangle$

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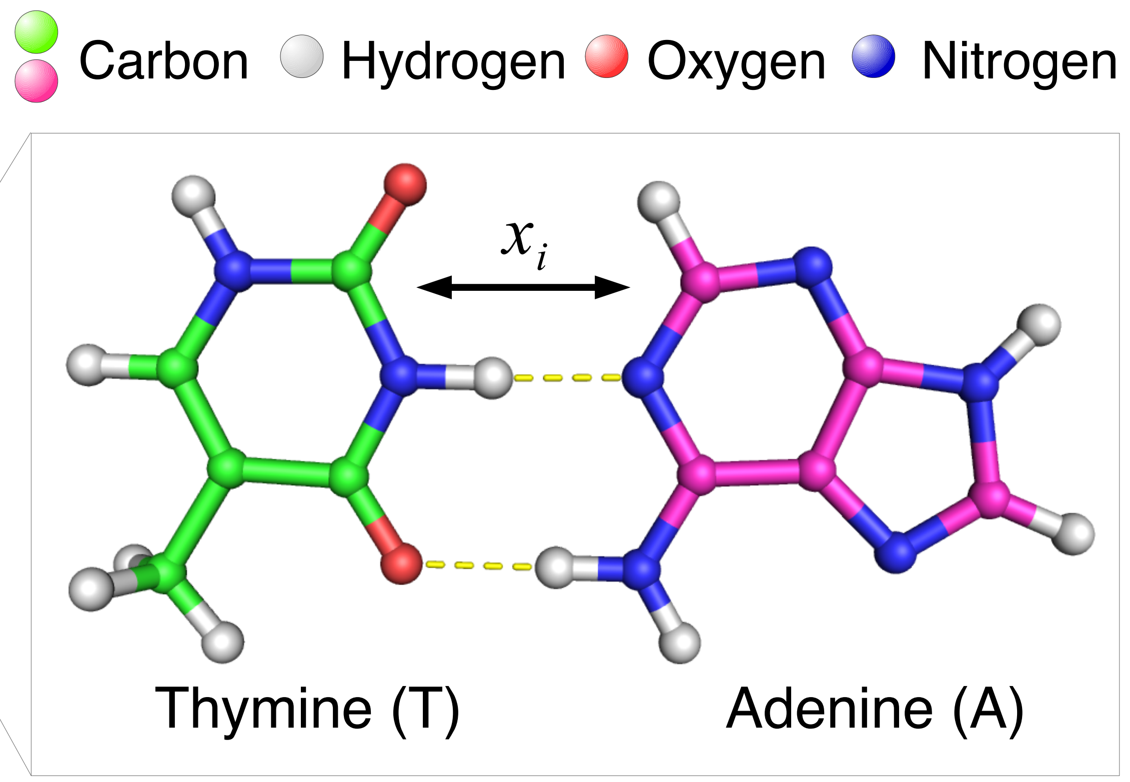
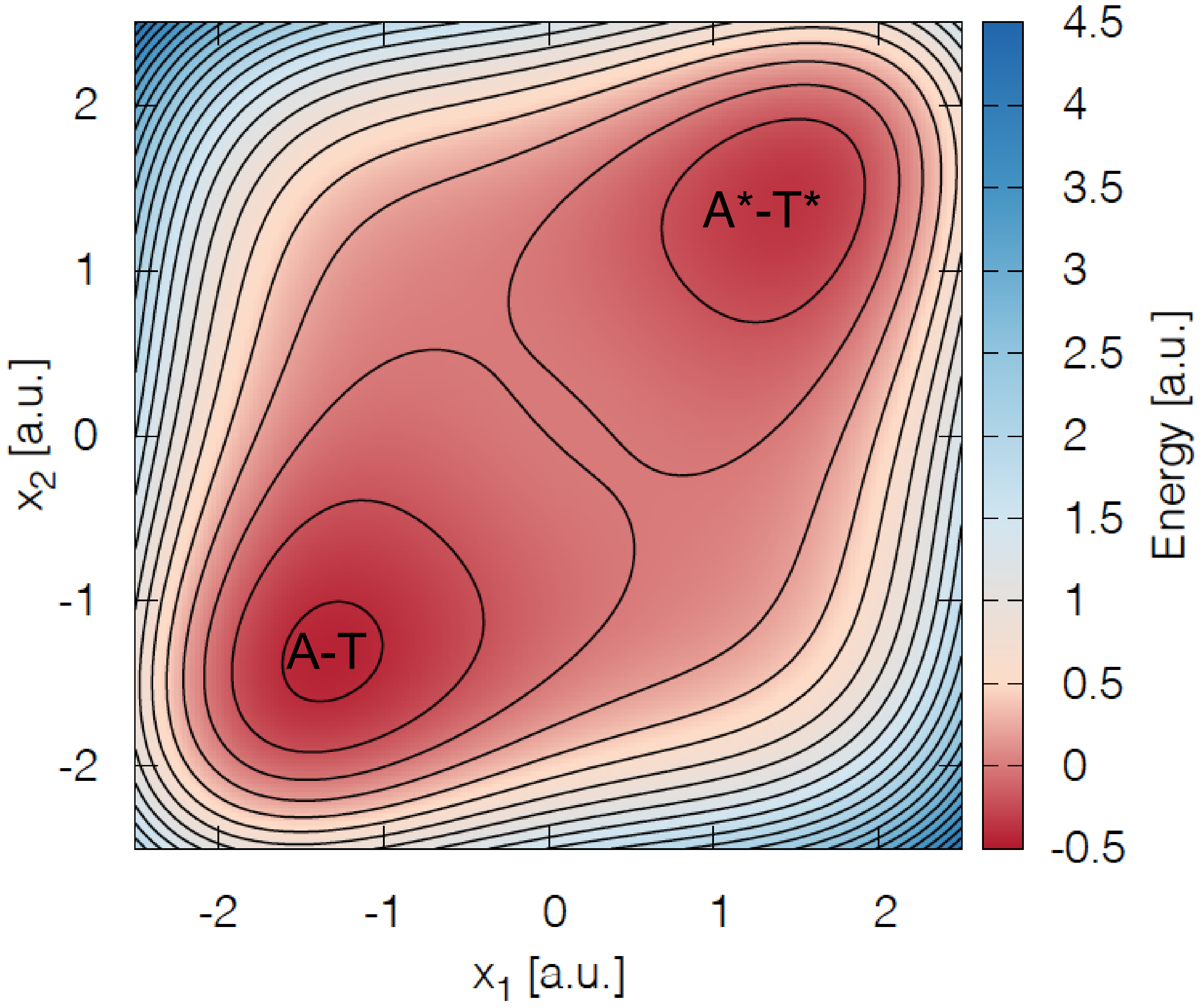
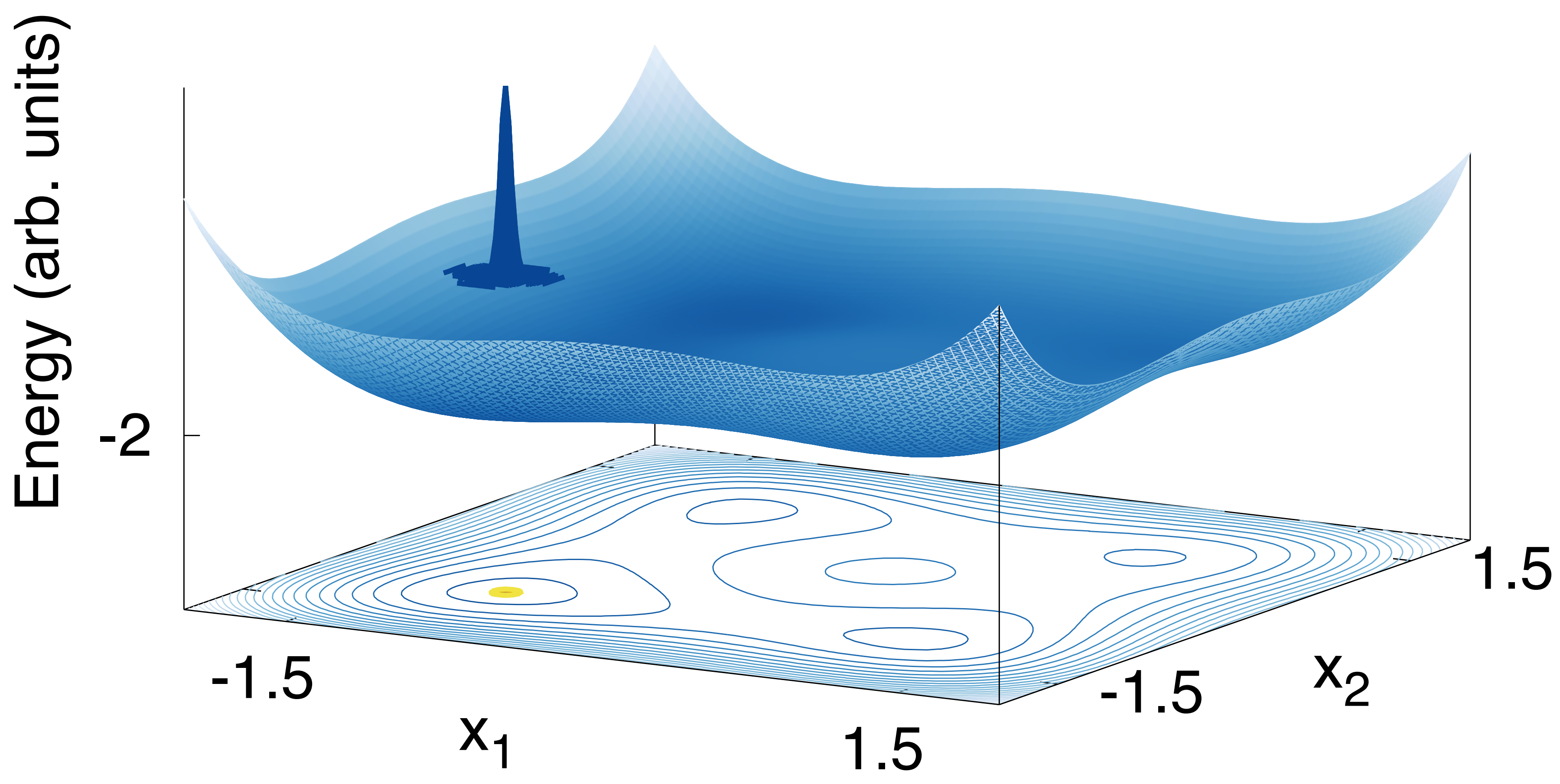
TENSOR-TRAIN ITERATIVE POWER ALGORITHM (IPA) FOR HYDROGEN BOND CONFIGURATIONS



Cut of Potential Energy Surface



Optimized Density



IPA enables identification of minimum energy molecular structure in up to

<u>**400 dimensions**</u>

beyond the capabilities of traditional grid-based approaches.

Micheline B. Soley, P. Bergold, A. A. Gorodetsky, V. S. Batista, JCTC, 17 (2021) 3280.

TENSOR-TRAIN IPA FOR PRIME FACTORIZATION OF

N=706851632784678312266808500466226101921669464385547527413569690763875796535401970800670478642897888271976359744482
562359245255871481739623795579868353636314461966874443074041408313128692006363959785724202562228073836999106855285692
644519543596165416986742134293741597127675540821848168930895358055666287697516694095534129648730690125043477471833212
349793956605095177438931303780173137245526404005011234493448949129910141059289267762650584326994153659208412726332997
462438687870054417384845219345545931344117340554314343141137650652780276322503358263710195619202289345940500455145744
883165448337677596088250881427571882314088881932567503546418747166615832389084594281762910485260868705276033961220609
224776095252926589540883980662468401888155270013513324524885486480997674192024201965727093108011252558162000937820818
289962114867981400584657710372992254661651075867403455271862309293906286499648242242986288787222152904308057485409954
533738370564925649123085757803987173118400940313676432083764110214364773166340998722735409974591180067191469076049004
990136642849972236687753072494237232352439460455688359872474591414017010339652063399874368946520524420895339479018793
070897634840285234432774742369999277850122336405790841422230843219659893780948617881279338270396619033205950196511316
257091358116322050813989056964945986023783919248741071072962269712626923426879258222092881844235635689133010595822918
984997483775345610409787261221110792047573908774977452473950325112788755615951458355928363904800199351760947325479155
433825636657097387649882679335732149029616430970902466976878151686416676123948749805195358784563373269368287844699081
416672704805301901168284431187235266294215540830234018607070261173839865411330806649094794367497678751782354249767965
655353869002681172964831857320702886587628275367562891236632051499981753839756599248211612276227322422314481323763460
724198651775643388900483543794055612391518556384941649274220842164411249318555909741938580116701236386843737520320663
510359674170467923211831676330352926714149993079607552107165280929146221890833003373014203637051377141516923445674118
786787019038337353114208013948310460978032954374272648638224882169487512573279160687585894629855333685604706409429556
528162697830179253939140163631691209891628750585199171480727149244103302709672451579009856352447655990913364831083058
733364543962544886341889094948465981128593596305804674031386494241068161689907124702782635437449783659077321465250447
489337455902640728012518915859962093979227459401522552702162993212784118890164246142115460631756231339365887330840484
169917017828763051420718501484749277817922055547639246132025665835862594509151025242869798254964873565372048920491700
2583939955697859360862764310036106686693705353525252656142323642791967328180835792001

2,773 DIGITS (MORE THAN 9,212 BITS)

NUMBER OF ITERATIONS

required to reach optimal result with 50% certainty (á la Grover's algorithm):

$$U = \mathrm{diag}(\lambda_2, \ldots, \lambda_2, \lambda_1, \lambda_2, \ldots, \lambda_2) \in \mathbb{R}^{n\times n}, \quad 0 < \lambda_2 < \lambda_1$$

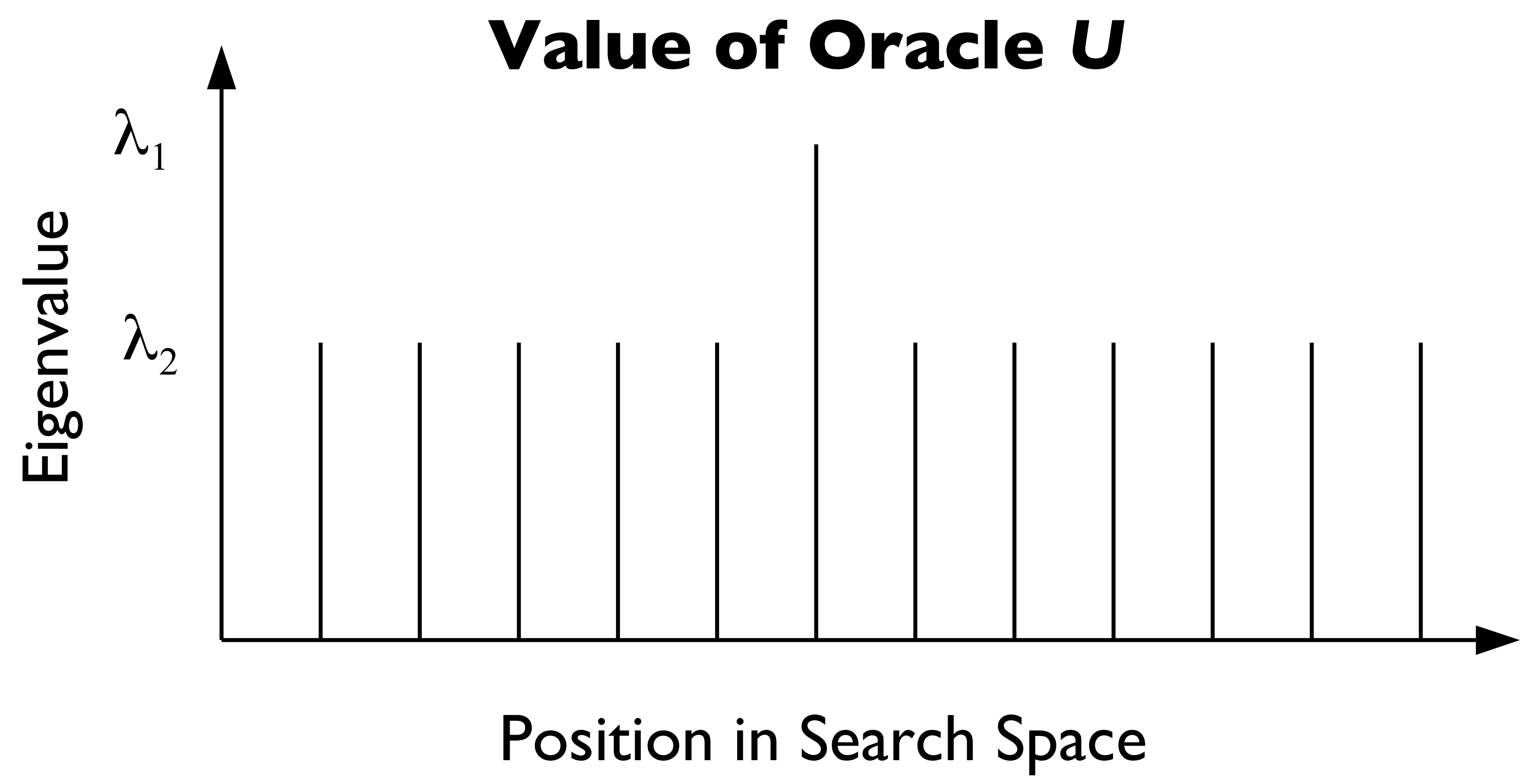
$$\rho_0 = \frac{1}{n}(1,\ldots,1) \in \mathbb{R}^n$$

$$\rho_k = \frac{\mathbf{U}^k \rho_0}{|\mathbf{U}^k \rho_0\|_1} \qquad \frac{\rho_{k,\,\min}}{\rho_{k,\,\max}} = \left(\frac{\lambda_2}{\lambda_1}\right)^k$$

$$1 = \|\rho_k\| = \rho_{k,\,\max} + (n-1)\rho_{k,\,\min}$$

$$\rho_{k,\,\max} = \frac{1}{1 + (n-1)\cdot(\lambda_2/\lambda_1)^k}$$

$$\frac{1}{2} \leq \frac{1}{1 + (n-1)\cdot(\lambda_2/\lambda_1)^k}$$



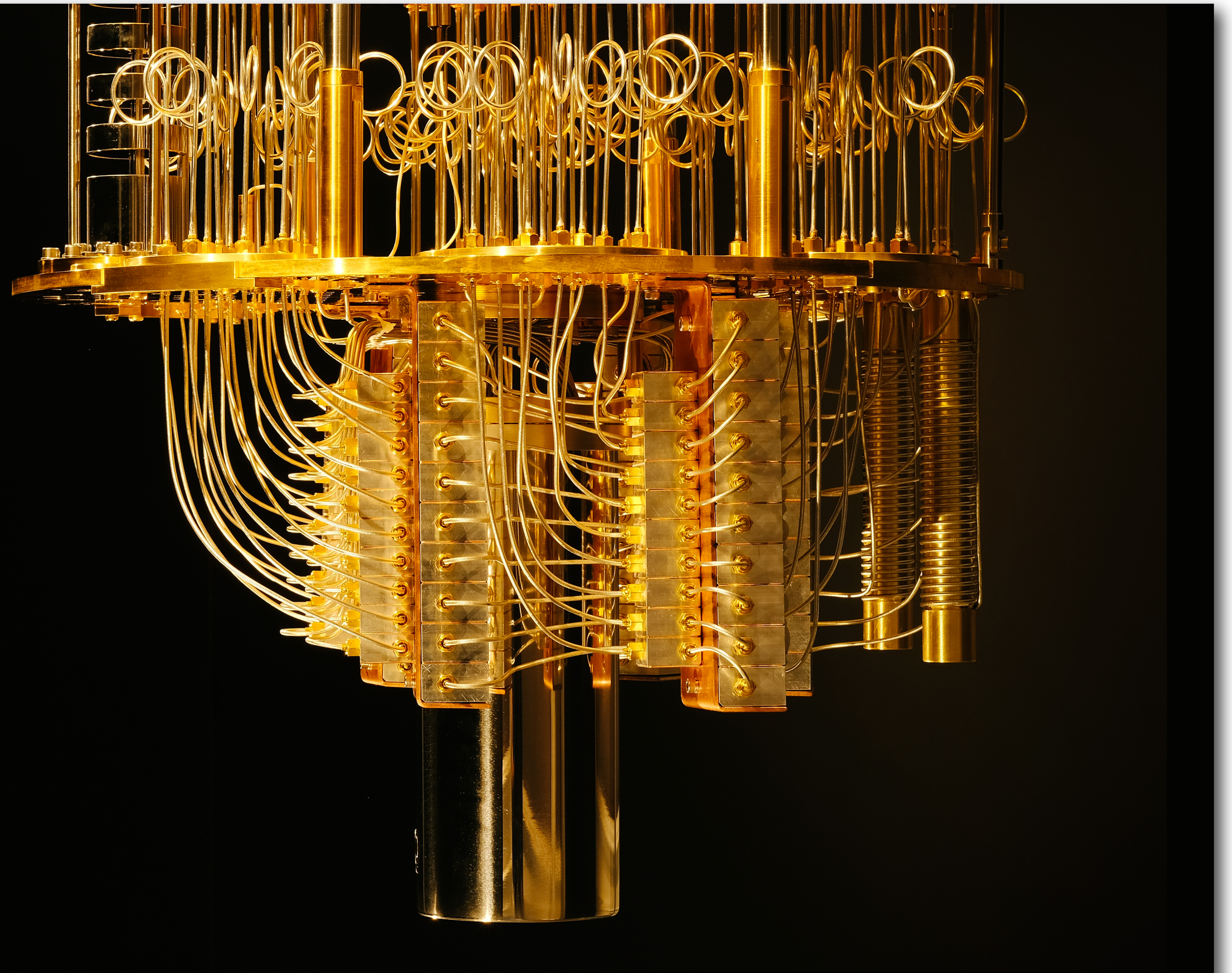
$$\boxed{k \geq \frac{\log(n-1)}{\log(\lambda_1/\lambda_2)}}$$

IPA requires fewer iterations than foremost quantum approach.

Micheline B. Soley, P. Bergold, V. S. Batista, JCTC 17 (2021) 3280.
L. K. Grover, Proceedings, 28th Annual ACM Symposium on the Theory of Computing, May 1996, 212.

TENSOR-TRAIN EFFICIENT QUANTUM COMPUTING ALGORITHMS FOR MOLECULAR SYSTEMS

This computational efficiency raises the question — can IPA be used to develop more efficient quantum computing algorithms for molecular systems?



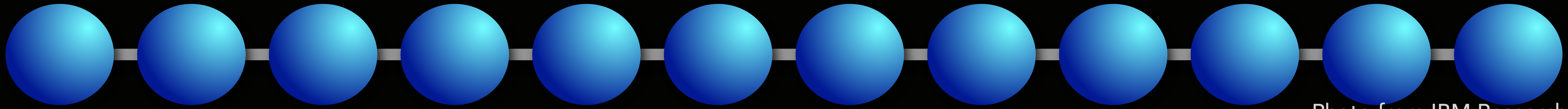
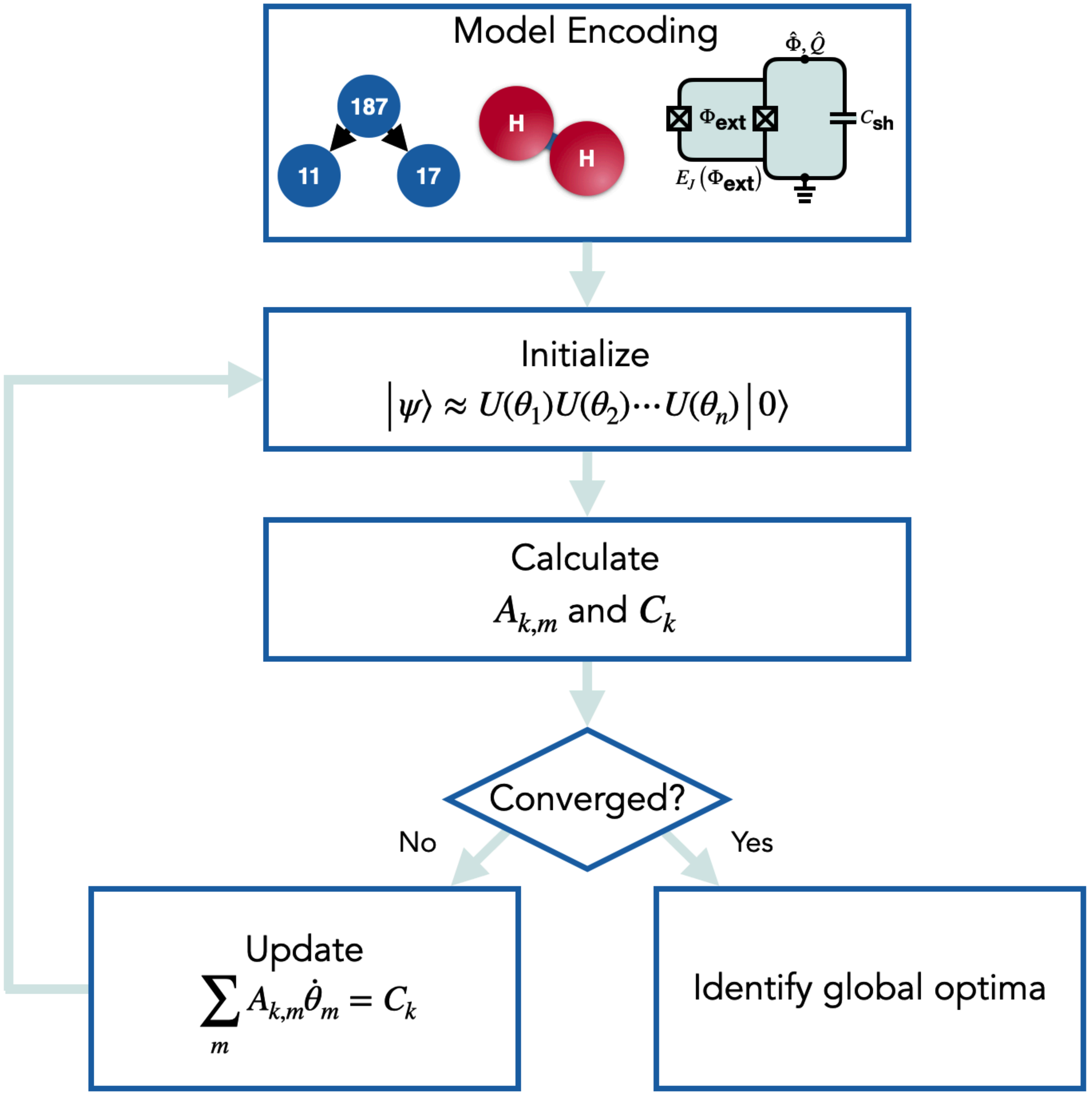


Photo from IBM Research.

T. H. Kyaw*, **Micheline B. Soley**,* B. Allen, P. Bergold, C. Sun, V. S. Batista, A. Aspuru-Guzik, (2022) arXiv:2208.10470v1.

F. Arute, et al. Science 369 (2020) 1084.

QUANTUM ITERATIVE POWER ALGORITHM (QIPA)



Connection to Cooling Schemes in Quantum Annealing

Accelerated Determination of Global Minima

First Instance of IPA on Quantum Computer

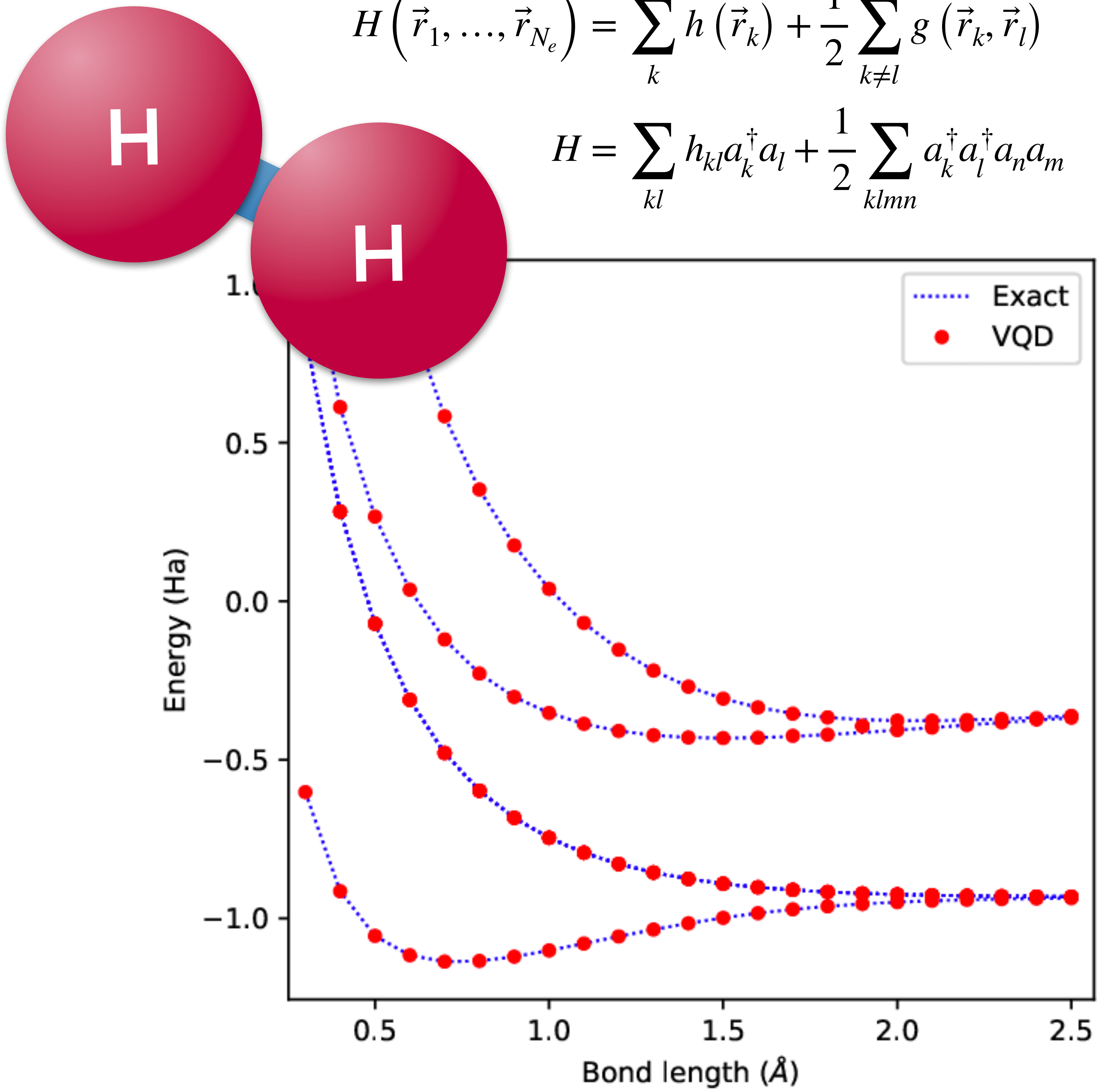
T. H. Kyaw*, **Micheline B. Soley**,* B. Allen, P. Bergold, C. Sun, V. S. Batista, A. Aspuru-Guzik, (2022) arXiv:2208.10470v1.

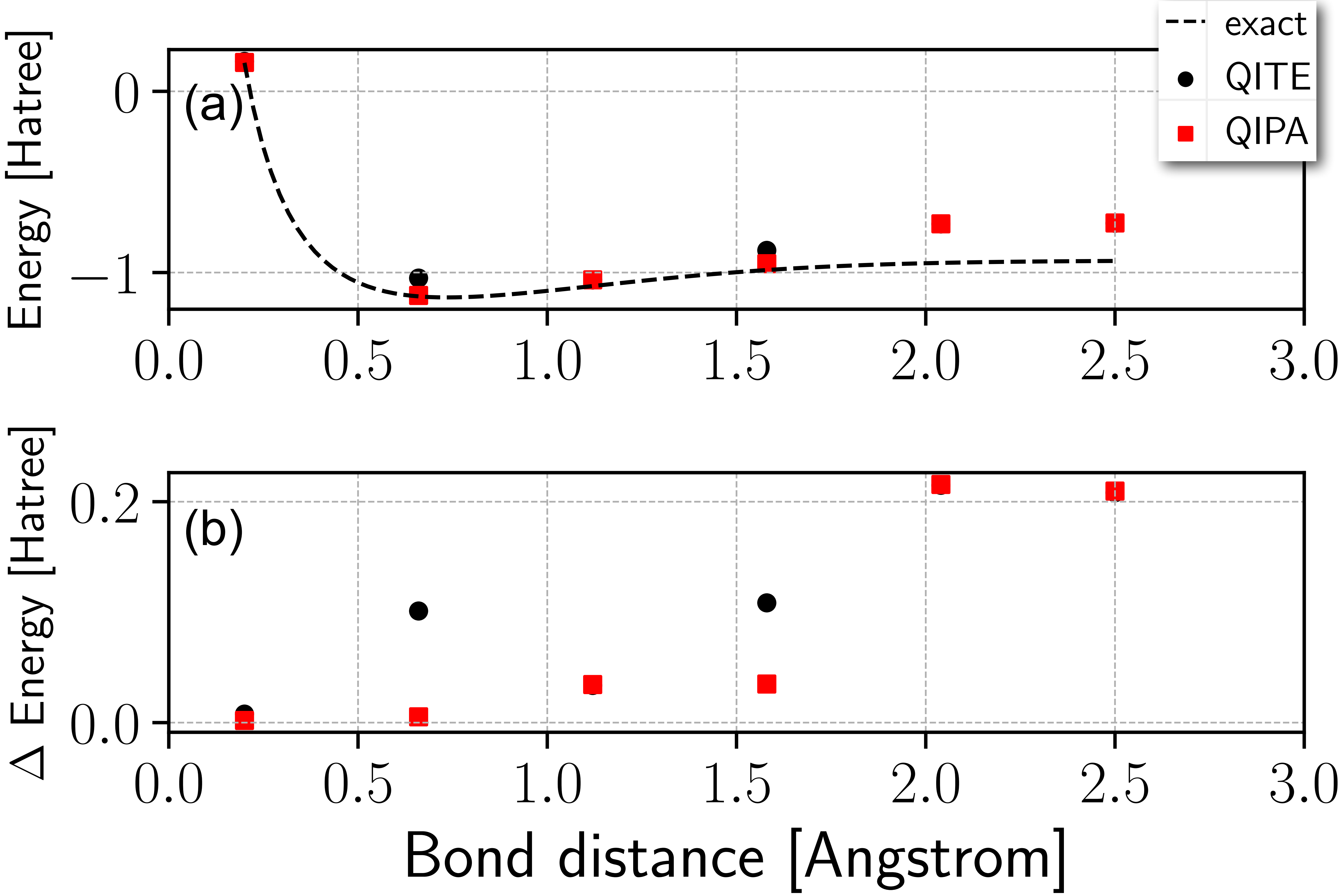
QIPA FOR ELECTRONIC STRUCTURE THEORY

QIPA **successfully** identifies the ground state energies of H_2 to high accuracy

$$H\left(\vec{r}_1, \ldots, \vec{r}_{N_e}\right) = \sum_{k}^{N_e} h\left(\vec{r}_k\right) + \frac{1}{2}\sum_{k \neq l}^{N_e} g\left(\vec{r}_k, \vec{r}_l\right)$$

$$H = \sum_{kl} h_{kl} a_k^\dagger a_l + \frac{1}{2}\sum_{klmn} a_k^\dagger a_l^\dagger a_n a_m$$

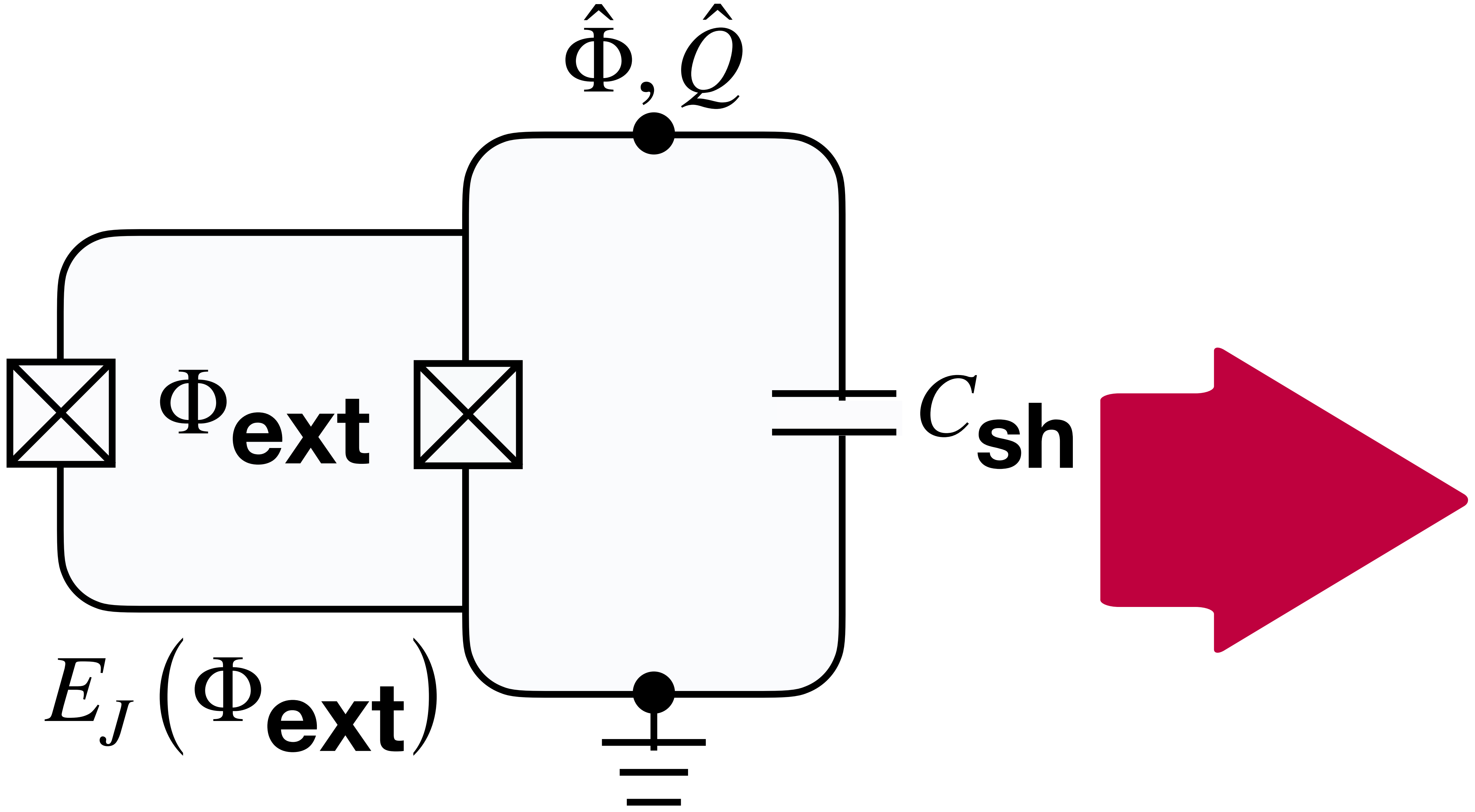




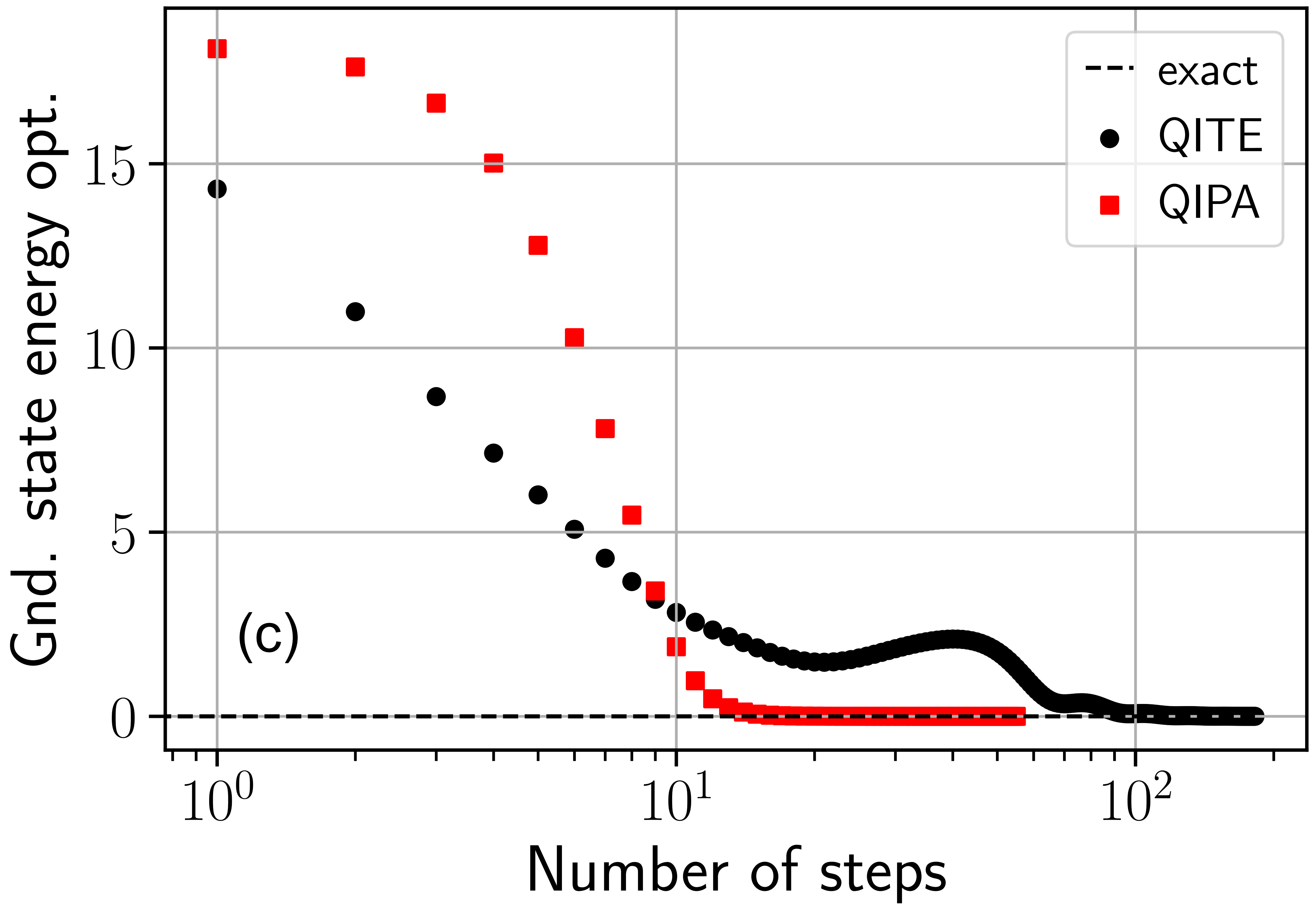
T. H. Kyaw*, **Micheline B. Soley**,* B. Allen, P. Bergold, C. Sun, V. S. Batista, A. Aspuru-Guzik, (2022) arXiv:2208.10470v1.

QIPA FOR QUANTUM COMPUTER DESIGN

First dynamical optimization of quantum processor design via quantum computing



$$\hat{H}_{M\text{-transmon}} = 2e^2 \sum_{i,j=1}^{M} \left(\mathbf{C}^{-1}\right)_{ij} \hat{N}_i \hat{N}_j - 2\sum_{i=1}^{M} E_{J,i} \left|\cos\left(2\pi f_i\right)\right| \cos\hat{\varphi}_i$$

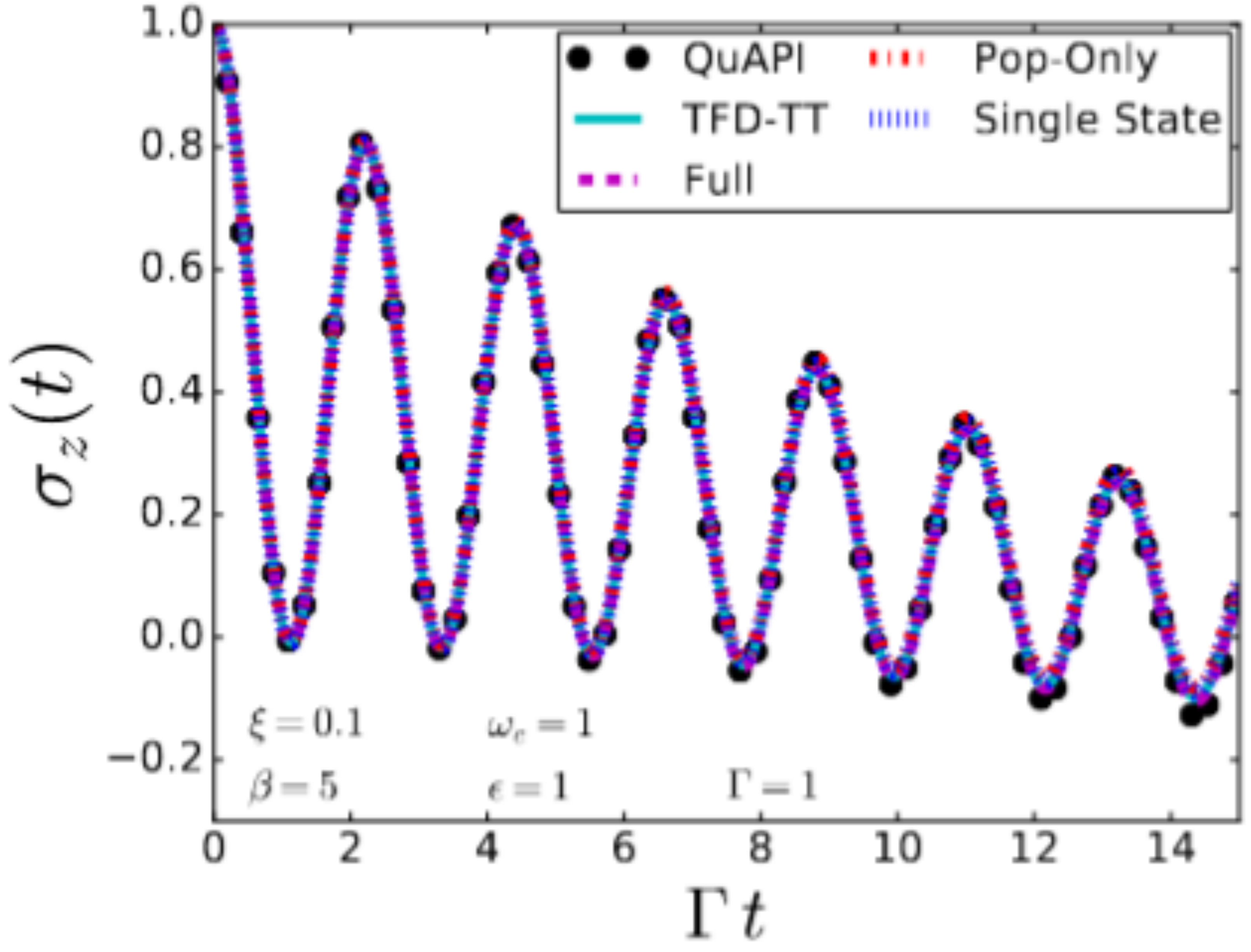


Advantage of QIPA over QITE for early steps over a broad parameter range

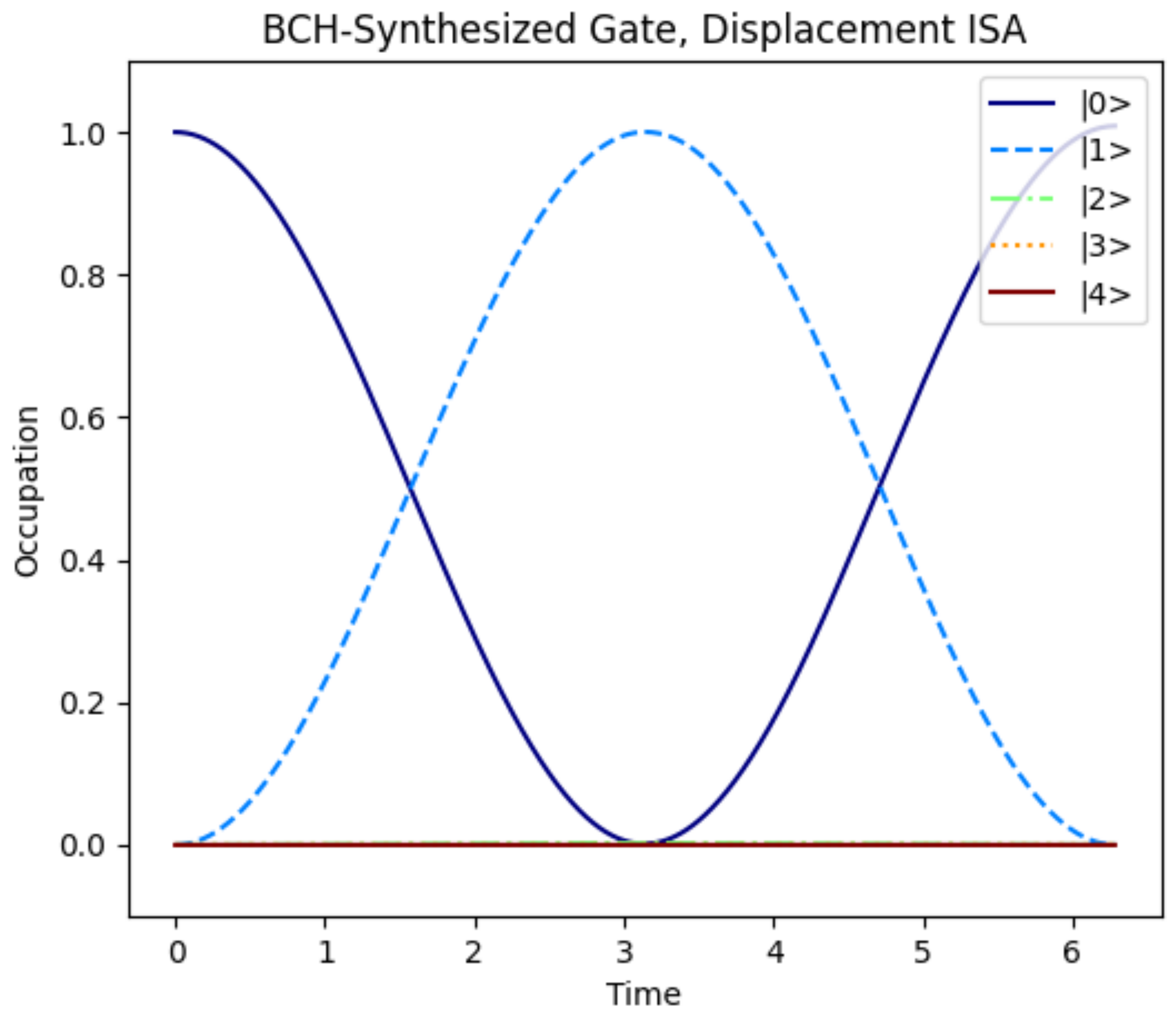
T. H. Kyaw*, **Micheline B. Soley**,* B. Allen, P. Bergold, C. Sun, V. S. Batista, A. Aspuru-Guzik, (2022) arXiv:2208.10470v1.
T. H. Kyaw,* Ti. Menke,* et al. (2021) arXiv:2006.03070v3.

APPLICATIONS OF TENSOR-NETWORK AND QUANTUM COMPUTING APPROACHES

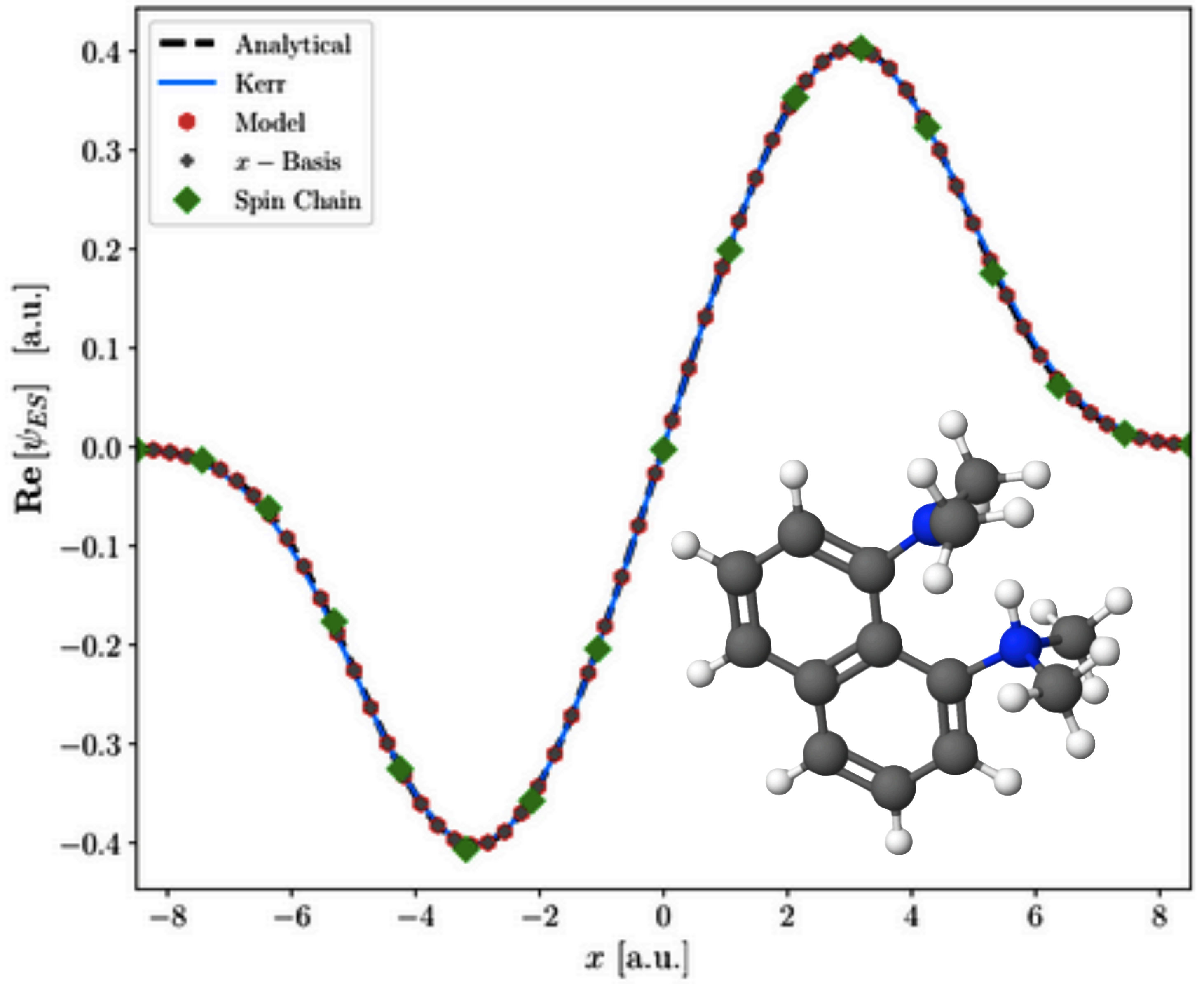
OPEN QUANTUM DYNAMICS



INSTRUCTION SET ARCHITECTURE



EIGENSTATE DETERMINATION METHOD



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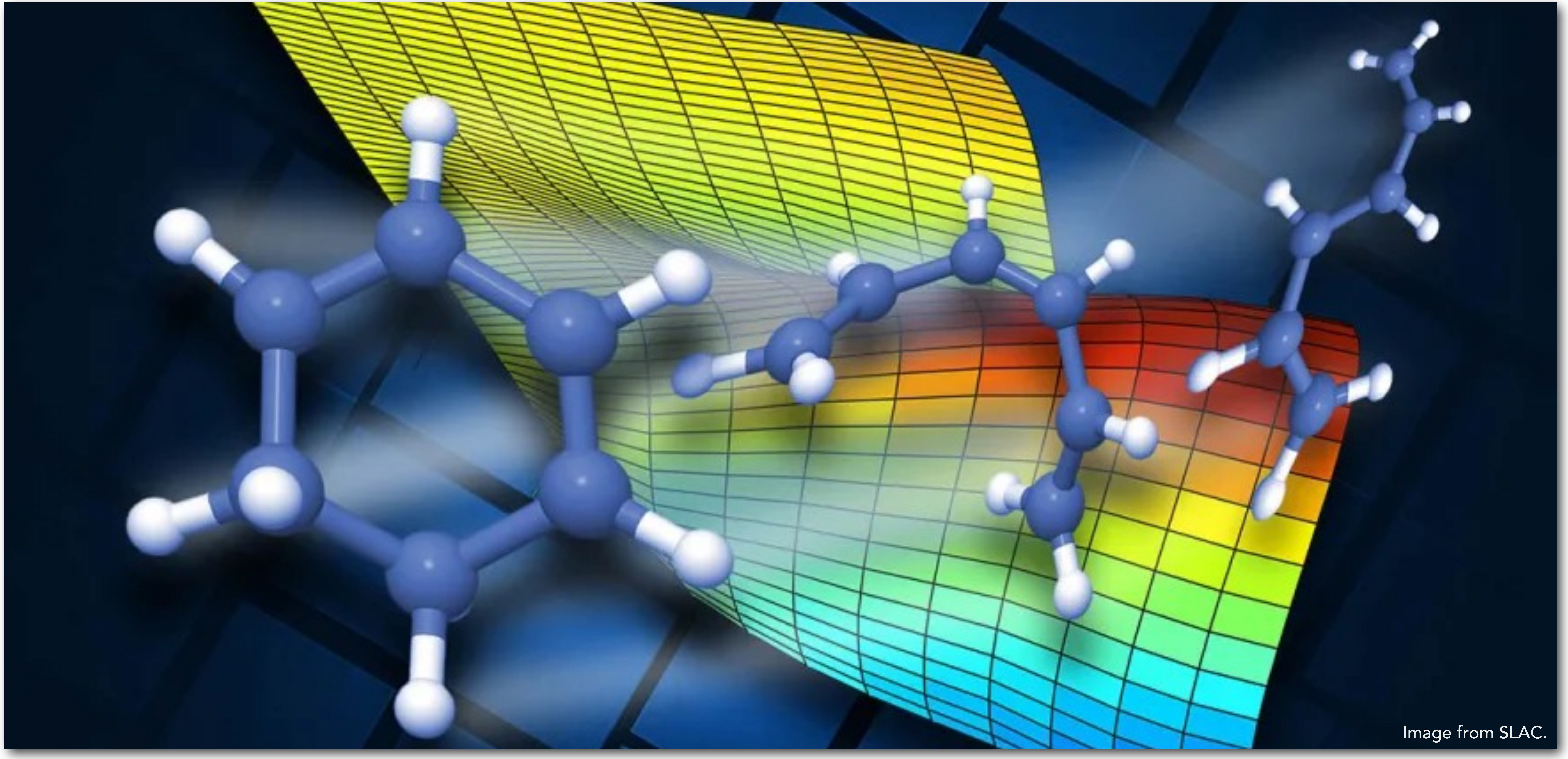
OUTLOOK

Tensor networks and quantum computers' efficiency and ability to enable exact quantum dynamics makes the method well-suited to a wide range of processes in chemistry beyond reach with standard grid-based methods.



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