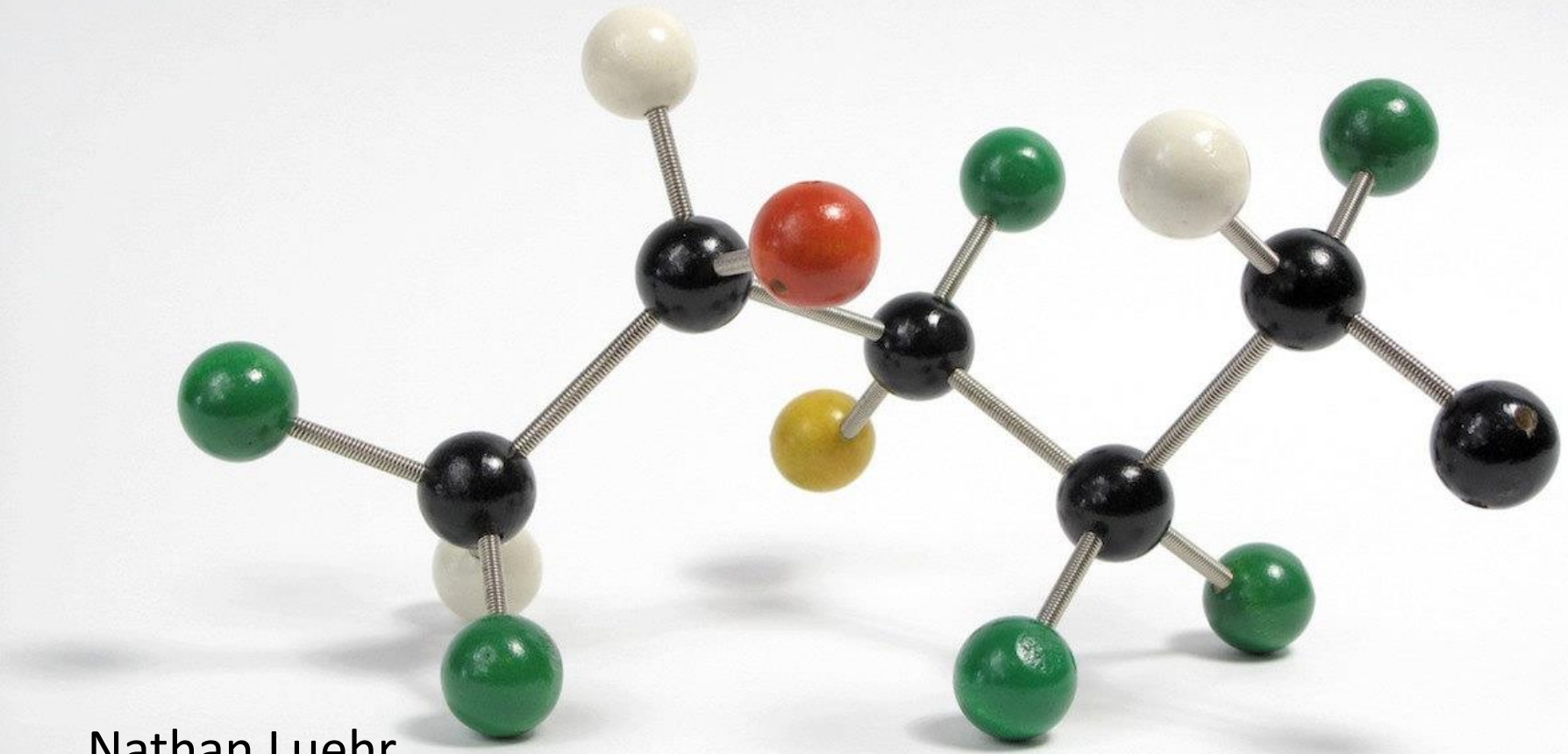
Interactive *ab initio* molecular dynamics



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A computational study of novel nitratoxycarbon, nitritocarbonyl, and nitrate compounds and their potential as high energy materials

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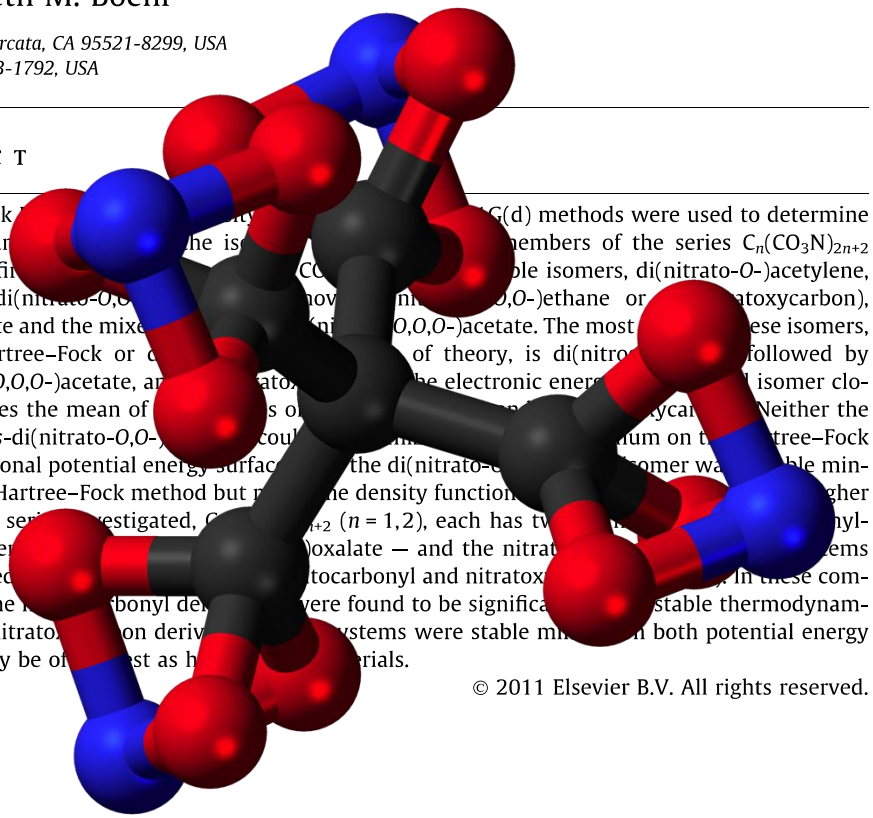
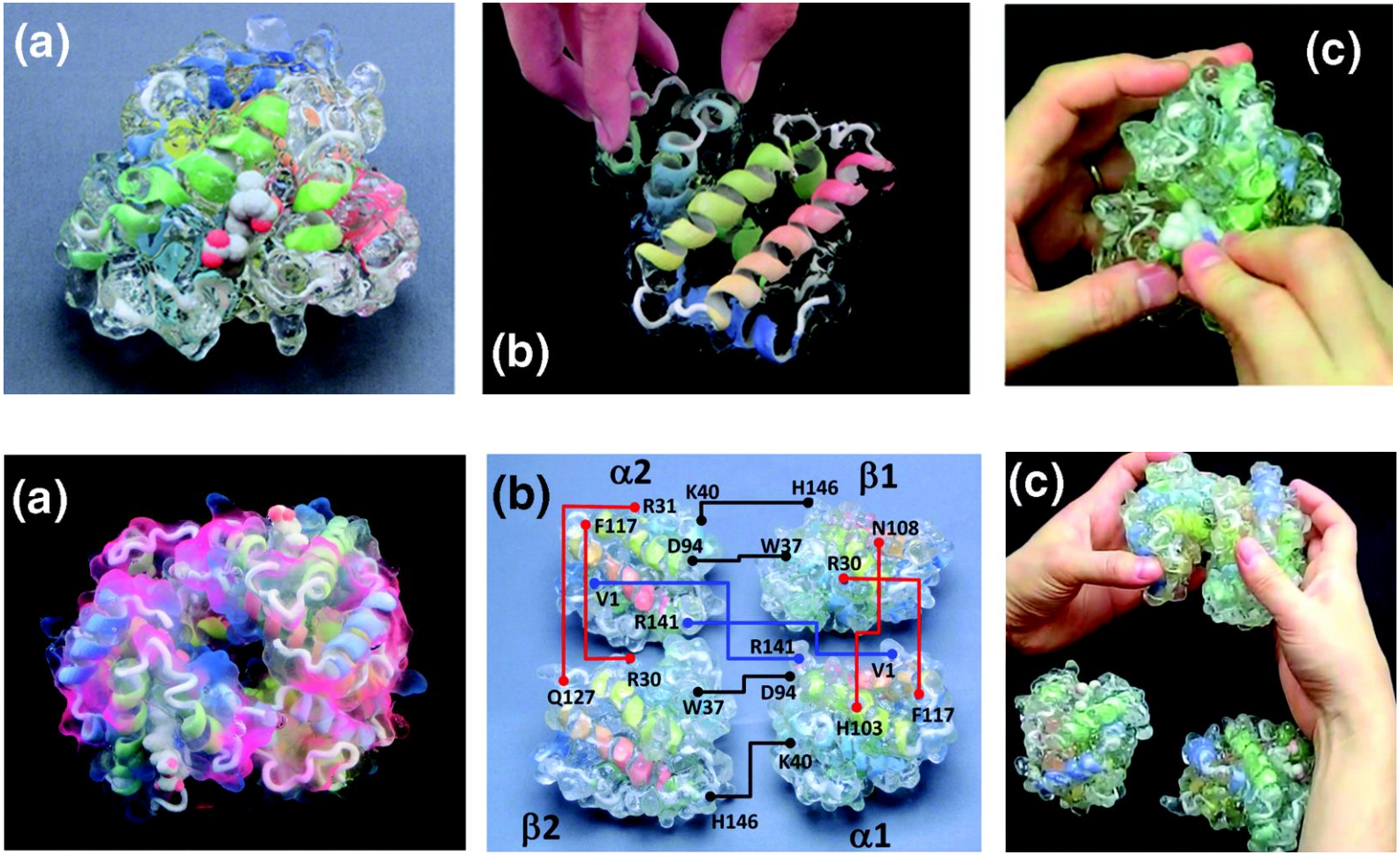
Density functional

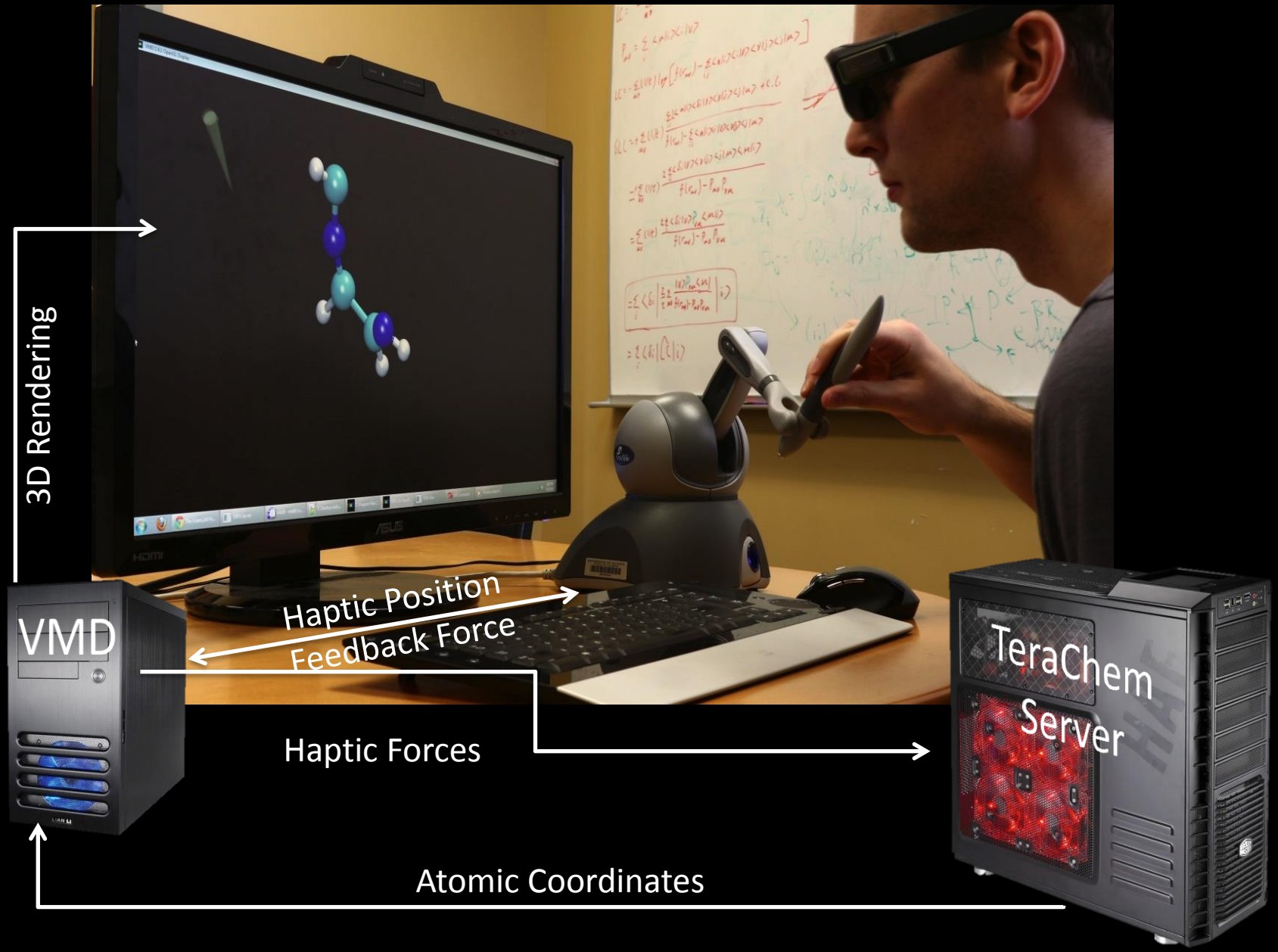
ABSTRACT

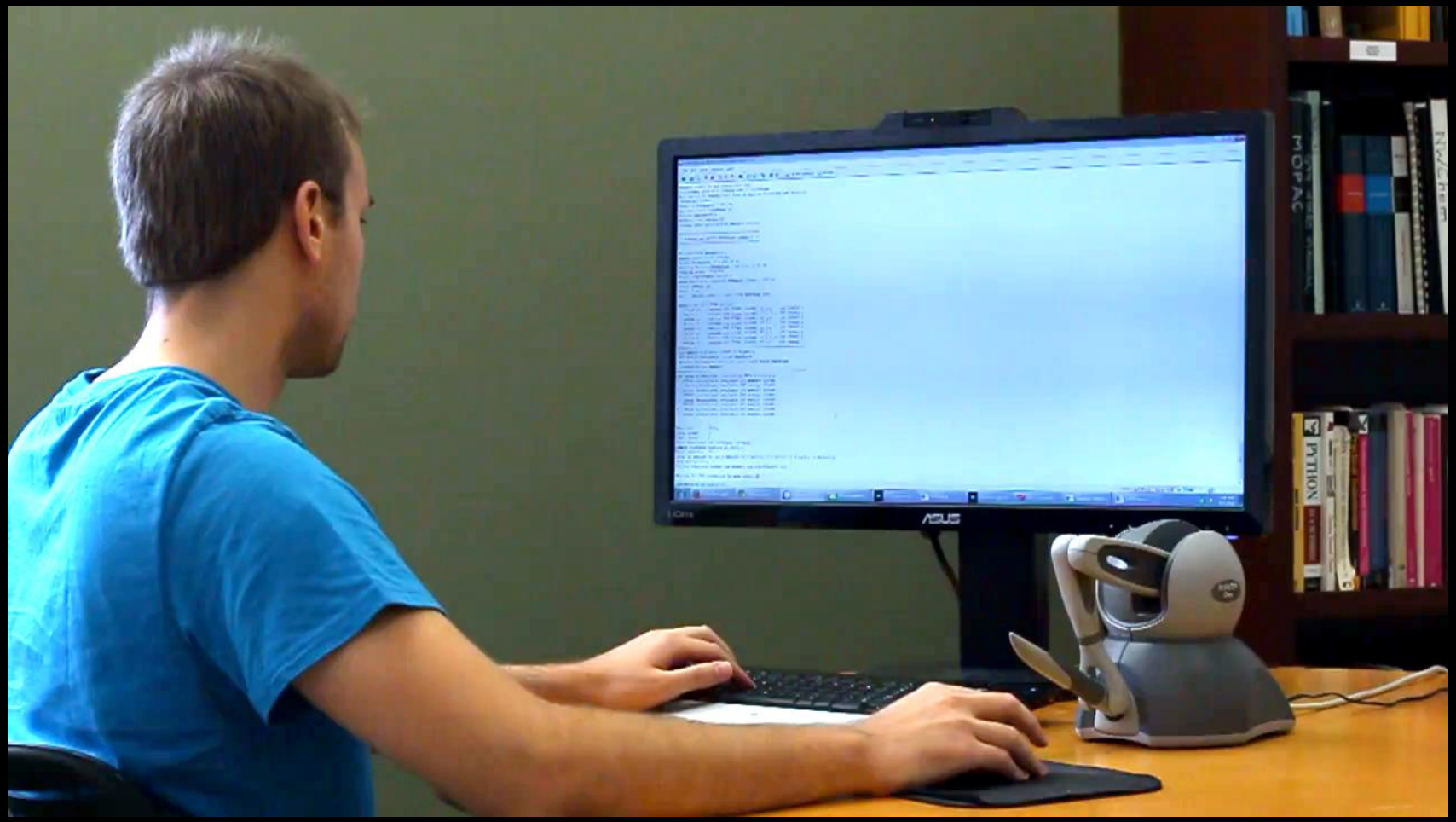
The Hartree–Fock [illegible]G(d) methods were used to determine the structures an[illegible]he is[illegible]embers of the series $C_n(CO_3N)_{2n+2}$ ($n = 0,1,2$). The fi[illegible]CO[illegible]ble isomers, di(nitrato-*O*-)acetylene, *cis*- and *trans*-di(nitrato-*O*,O[illegible]nov[illegible]n[illegible]*O*,*O*-)ethane or [illegible]atoxycarbon), di(nitroso)oxalate and the mixe[illegible]ni[illegible]*O*,*O*,*O*-)acetate. The most [illegible]ese isomers, both at the Hartree–Fock or d[illegible] of theory, is di(nitro[illegible]followed by nitroso(nitrato-*O*,*O*,*O*-)acetate, ar[illegible]ato[illegible]he electronic ener[illegible]l isomer closely approximates the mean of [illegible]s o[illegible]ycar[illegible]Neither the *cis*- nor the *trans*-di(nitrato-*O*,*O*-[illegible]coul[illegible]m[illegible]um on t[illegible]tree–Fock or density functional potential energy surfac[illegible]the di(nitrato-e[illegible]somer wa[illegible]ble minimum with the Hartree–Fock method but n[illegible]e density function[illegible]gher members of the ser[illegible]vestigated, C[illegible]$_{n+2}$ ($n = 1,2$), each has tw[illegible]nyl-substituted syste[illegible])oxalate — and the nitrat[illegible]ems (neglecting mixed[illegible]tocarbonyl and nitratox[illegible], In these compounds, while the [illegible]bonyl de[illegible]ere found to be significa[illegible]stable thermodynamically than the nitrato[illegible]on deriv[illegible]ystems were stable mi[illegible]n both potential energy surfaces and may be of[illegible]st as h[illegible]erials.



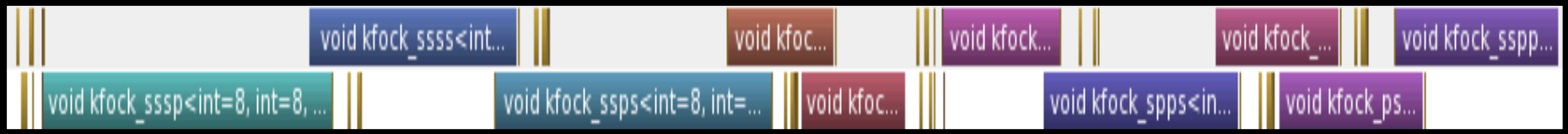


Masaru Kawakami. *Review of Scientific Instruments*, 2012; 83 (8): 084303

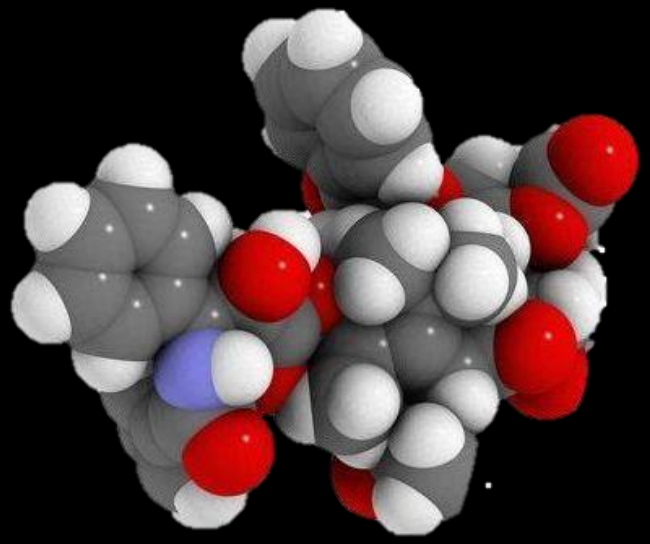

3D Rendering
VMD
Haptic Position
Feedback Force
Haptic Forces
TeraChem
Server
Atomic Coordinates

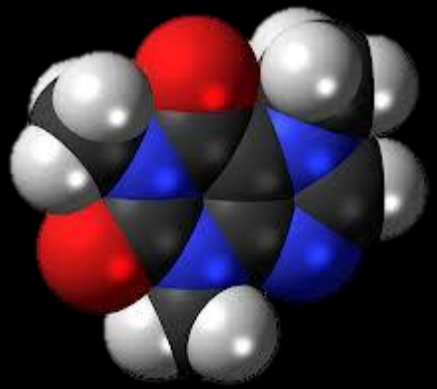

MOPAC
ASUS

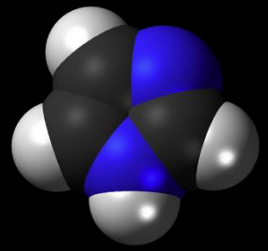
TeraChem Performance & Optimization



Molecule	Atoms	STO-3G	6-31G*
Imidazole	9	48 ms	287 ms
Caffeine	24	225 ms	1285 ms
Taxol	110	4297 ms	26.0 sec





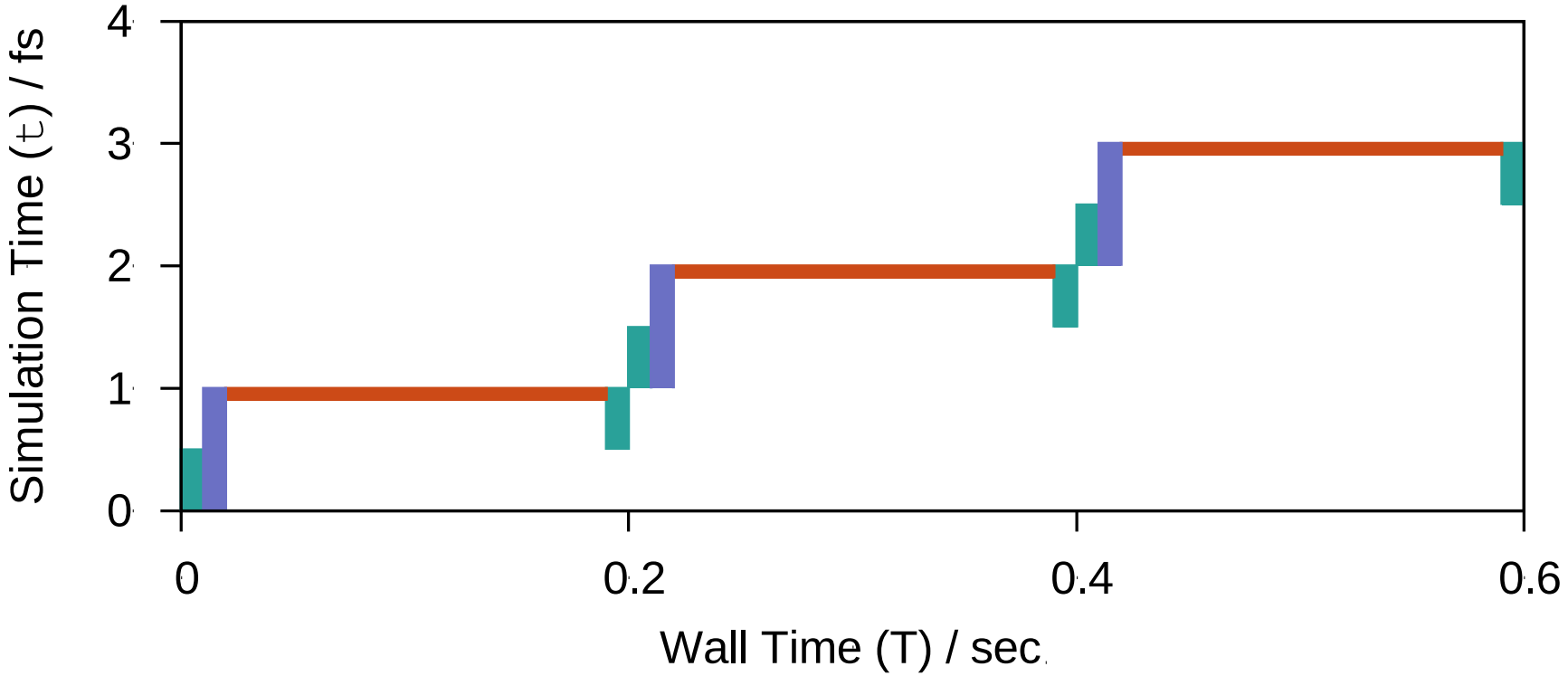


Verlet Integrator

$$v \leftarrow v + a^{AI}\frac{\Delta\tau}{2}$$

$$x \leftarrow x + v\Delta\tau$$

$$a_i^{AI} \leftarrow -\frac{\nabla_i E^{AI}(x)}{m_i}$$



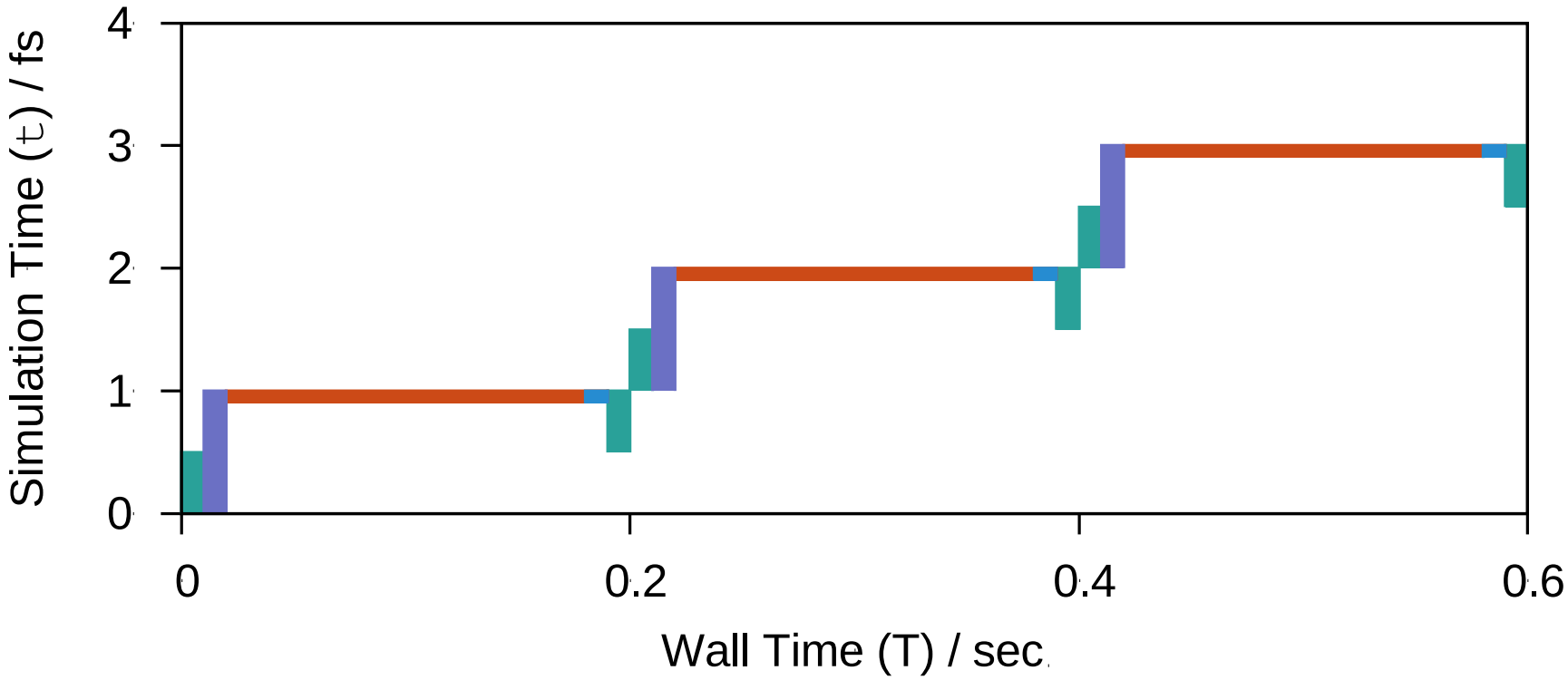
Naïve Haptic Integrator

$$a^{AI} \leftarrow -\frac{\nabla_i E^{AI}(x)}{m}$$

$$a^{H} \leftarrow \frac{haptic(T)}{m}$$

$$v \leftarrow v + (a^{AI} + a^{H})\frac{\Delta\tau}{2}$$

$$x \leftarrow x + v\Delta\tau$$



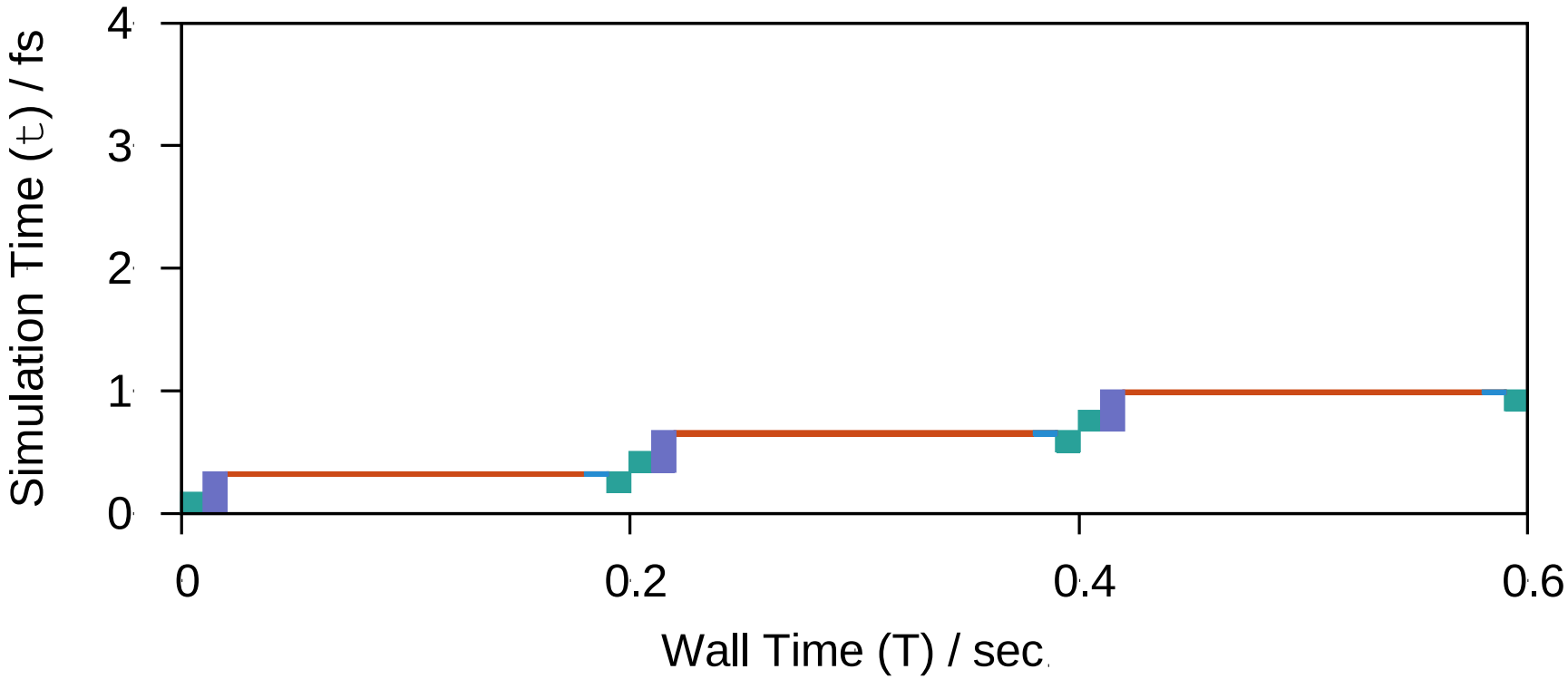
Naïve Haptic Integrator

$$a^{AI} \leftarrow -\frac{\nabla_i E^{AI}(x)}{m}$$

$$a^{H} \leftarrow \frac{haptic(T)}{m}$$

$$v \leftarrow v + (a^{AI} + a^{H})\frac{\Delta\tau}{2}$$

$$x \leftarrow x + v\Delta\tau$$



Haptic MTS Integrator

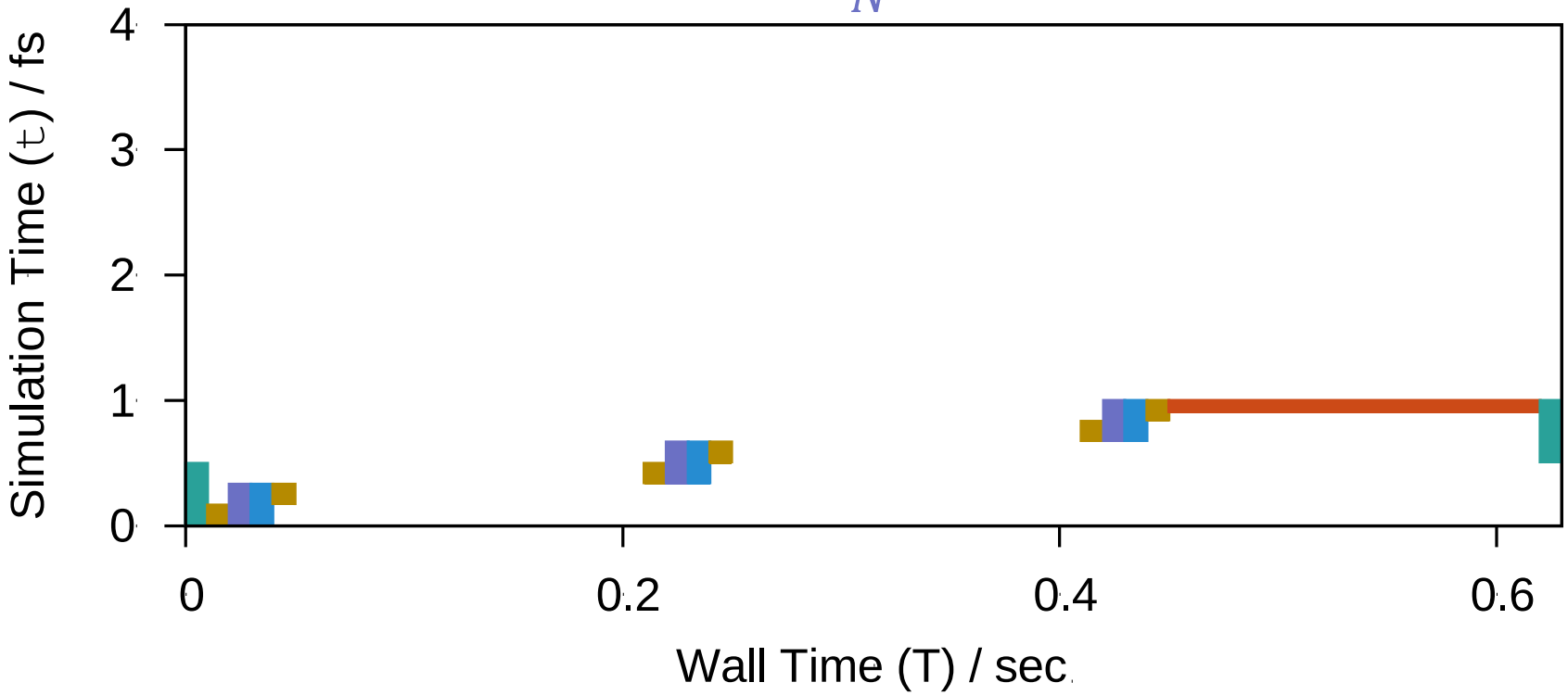
$$a^{AI} \leftarrow -\frac{\nabla_i E^{AI}(x)}{m}$$

$$a^{H} \leftarrow \frac{haptic(T)}{m}$$

$$v \leftarrow v + a^{AI}\frac{\Delta\tau}{2}$$

$$v \leftarrow v + a^{H}\frac{\Delta\tau}{2N}$$

$$x \leftarrow x + v\frac{\Delta\tau}{N}$$



Haptic MTS Integrator

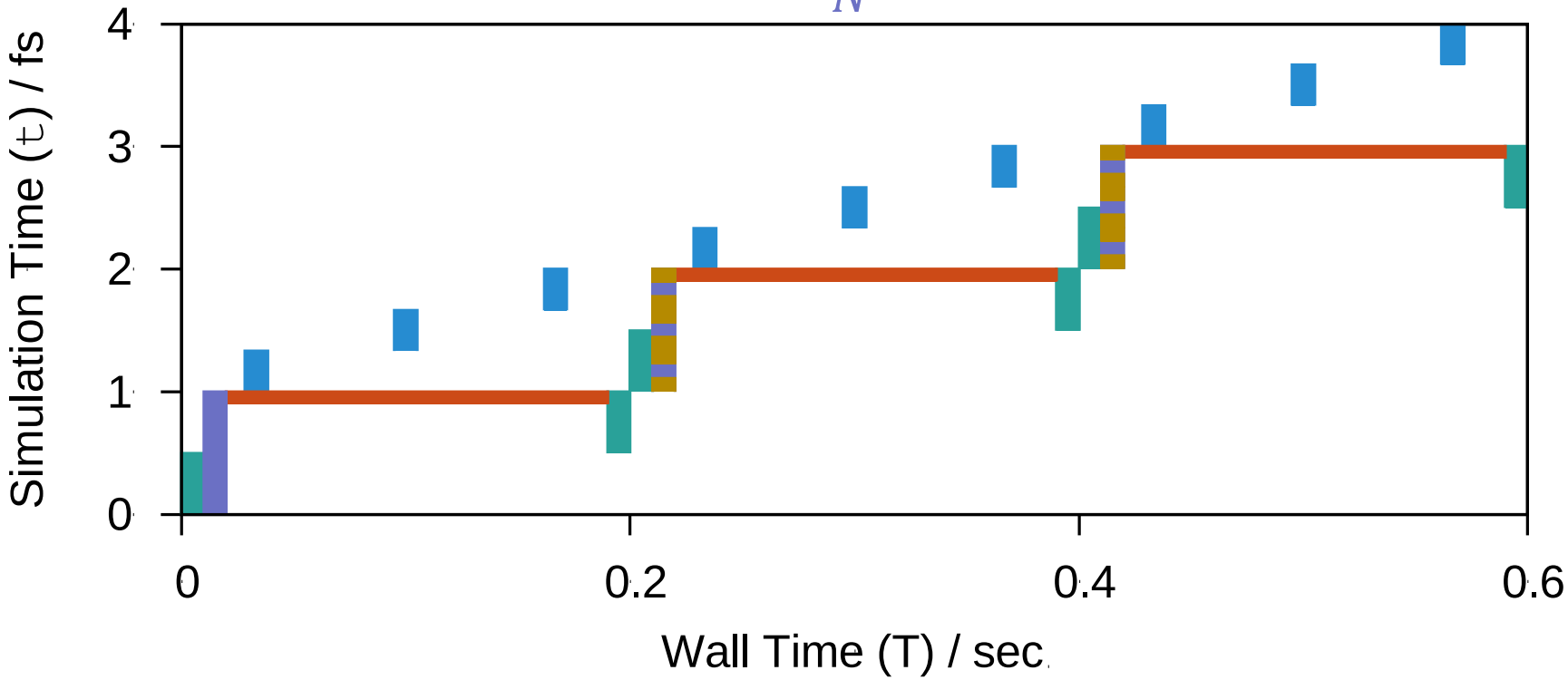
$$a^{AI} \leftarrow -\frac{\nabla_i E^{AI}(x)}{m}$$

$$a^{H} \leftarrow \frac{haptic(T)}{m}$$

$$v \leftarrow v + a^{AI}\frac{\Delta\tau}{2}$$

$$v \leftarrow v + a^{H}\frac{\Delta\tau}{2N}$$

$$x \leftarrow x + v\frac{\Delta\tau}{N}$$

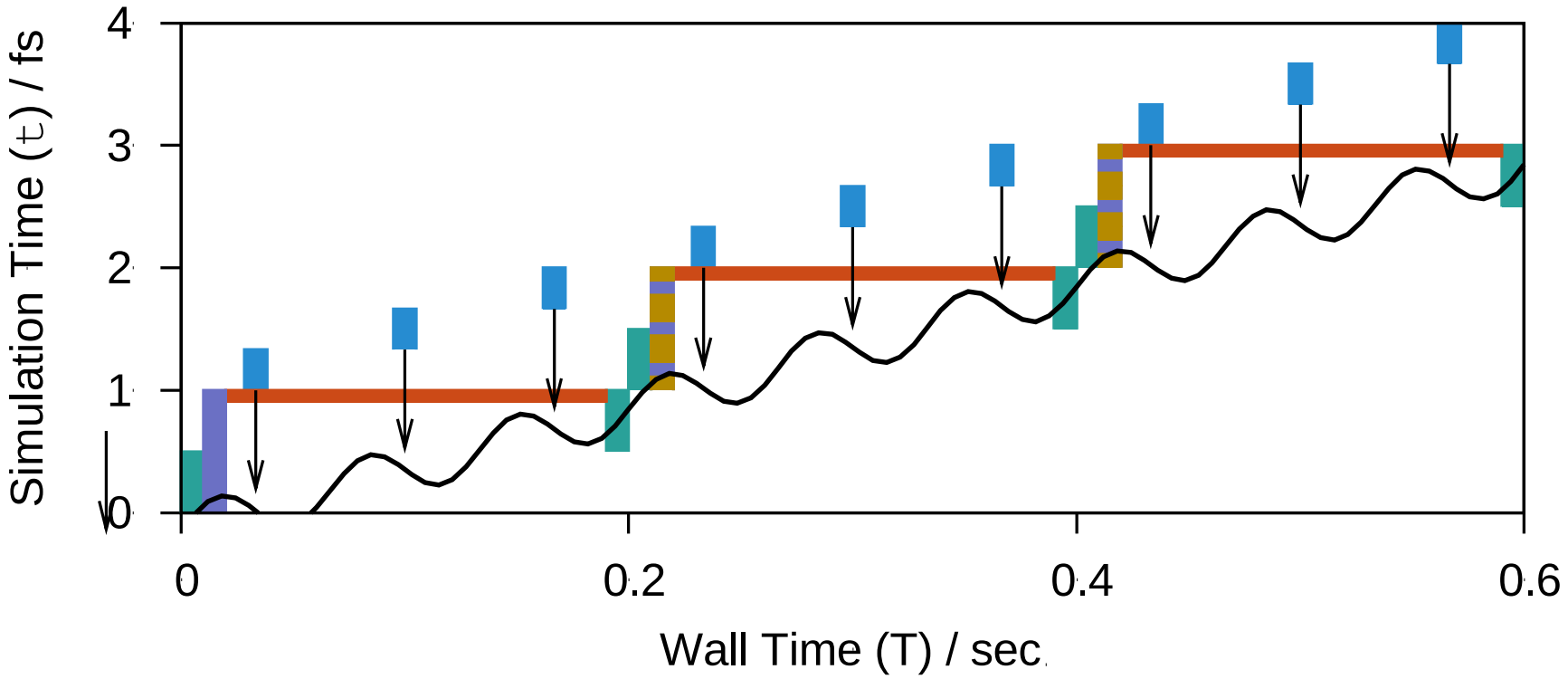


Piecewise Interpolation

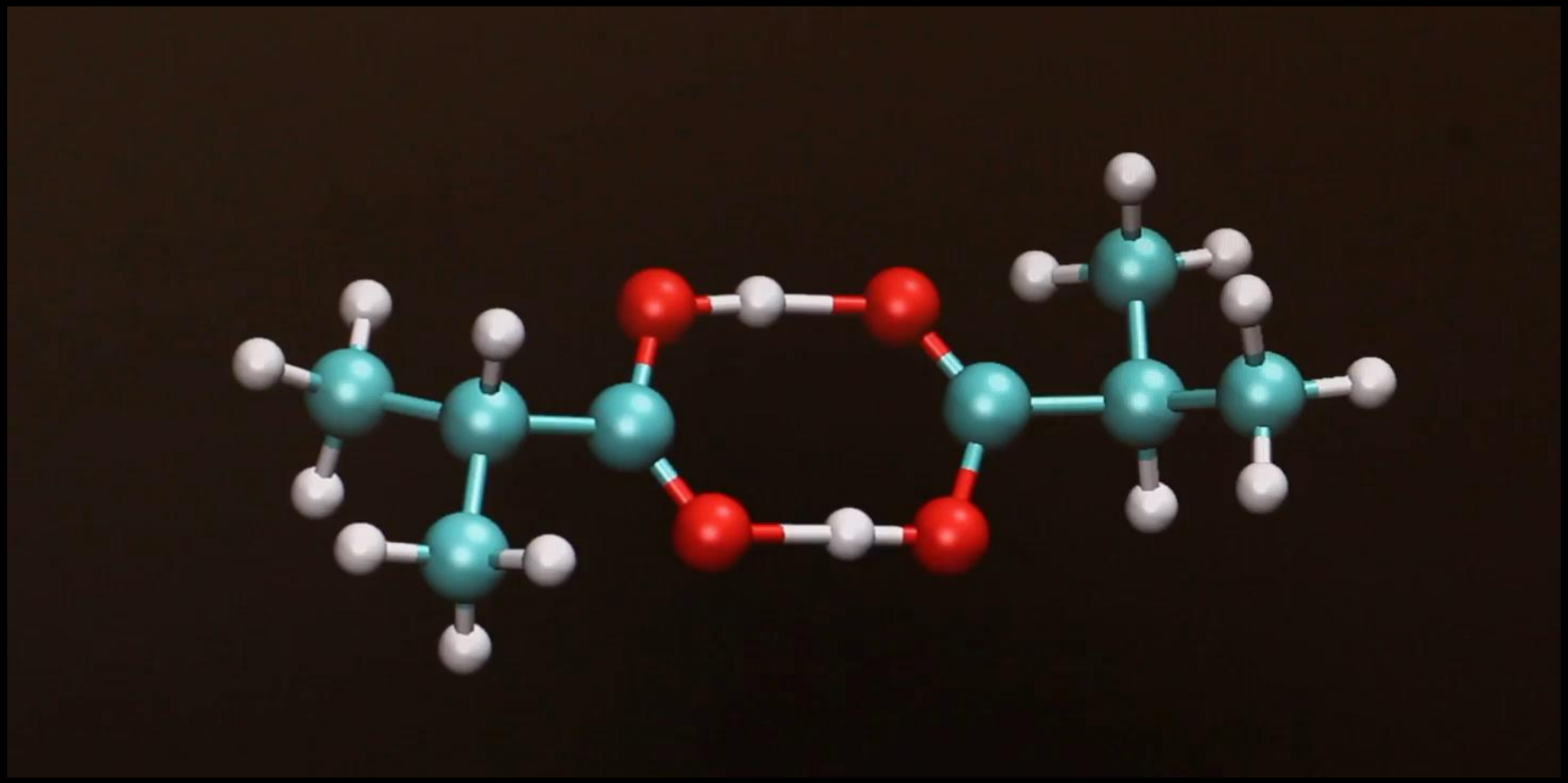
Pseudo-system

$$\tilde{v}(T) = \begin{cases} \dfrac{x(n\Delta\tau) - \tilde{x}(n\delta T)}{\delta T} & if\ T == n\delta T \\ \tilde{v}(T - \delta T) + haptic(T)\delta T & otherwise \end{cases}$$

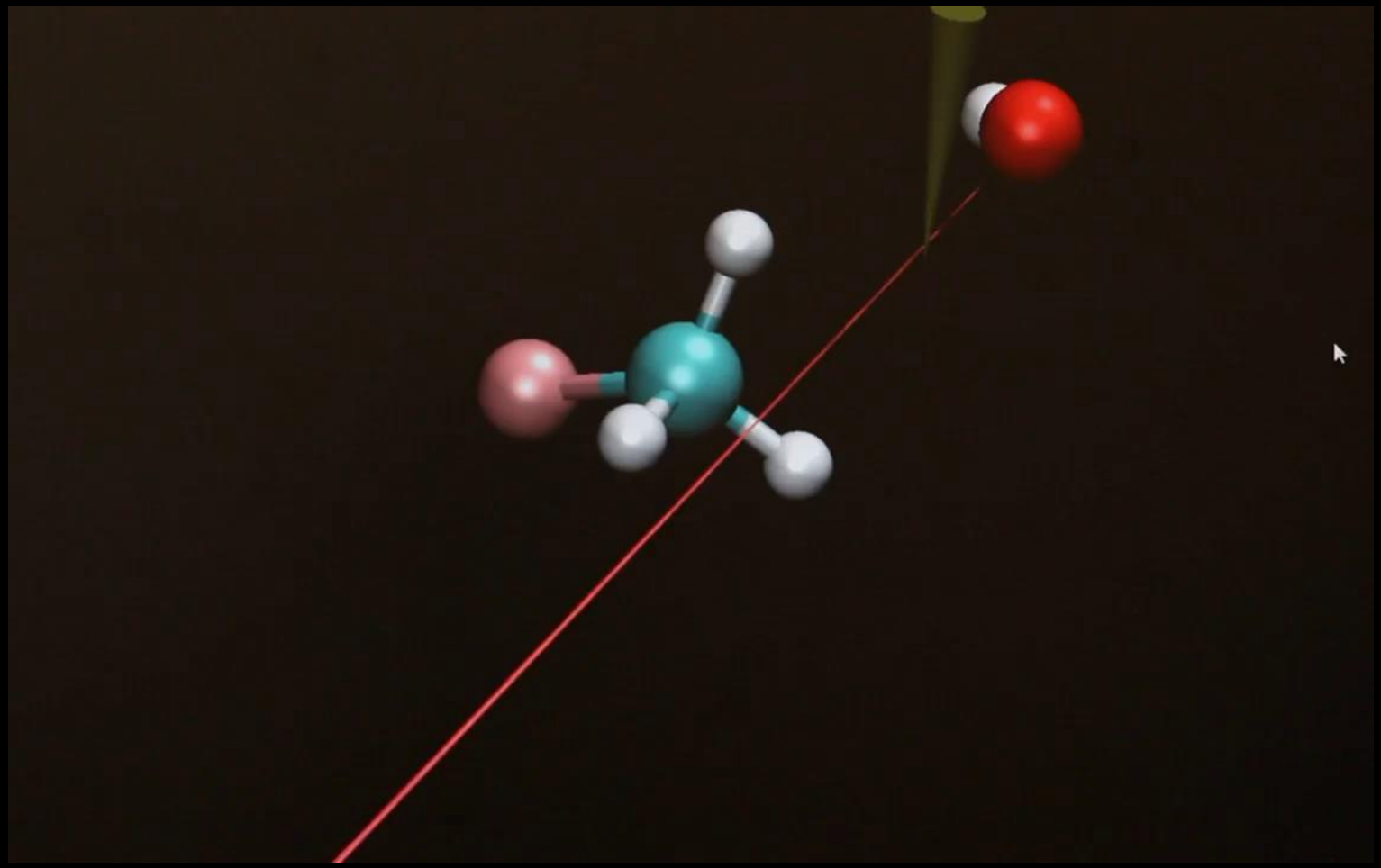
$$\tilde{x}(T) = \tilde{x}(T - \delta T) + \tilde{v}(T)\delta T + \frac{1}{2}h(T)\delta T^2$$



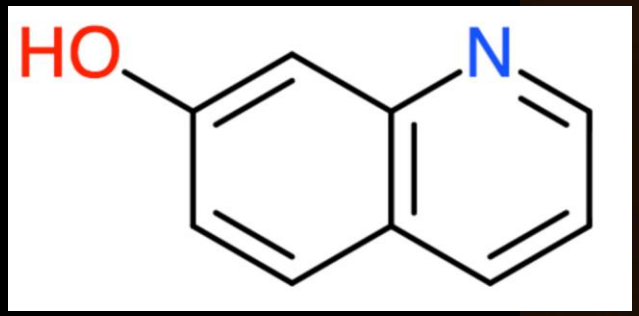
Ex1: Acid Dimer



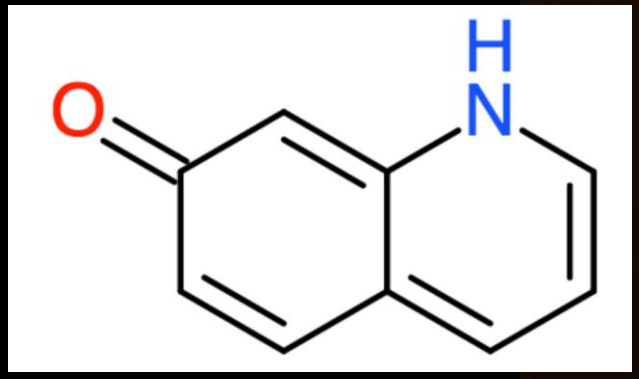
Ex2: $CH_3F + OH^-$

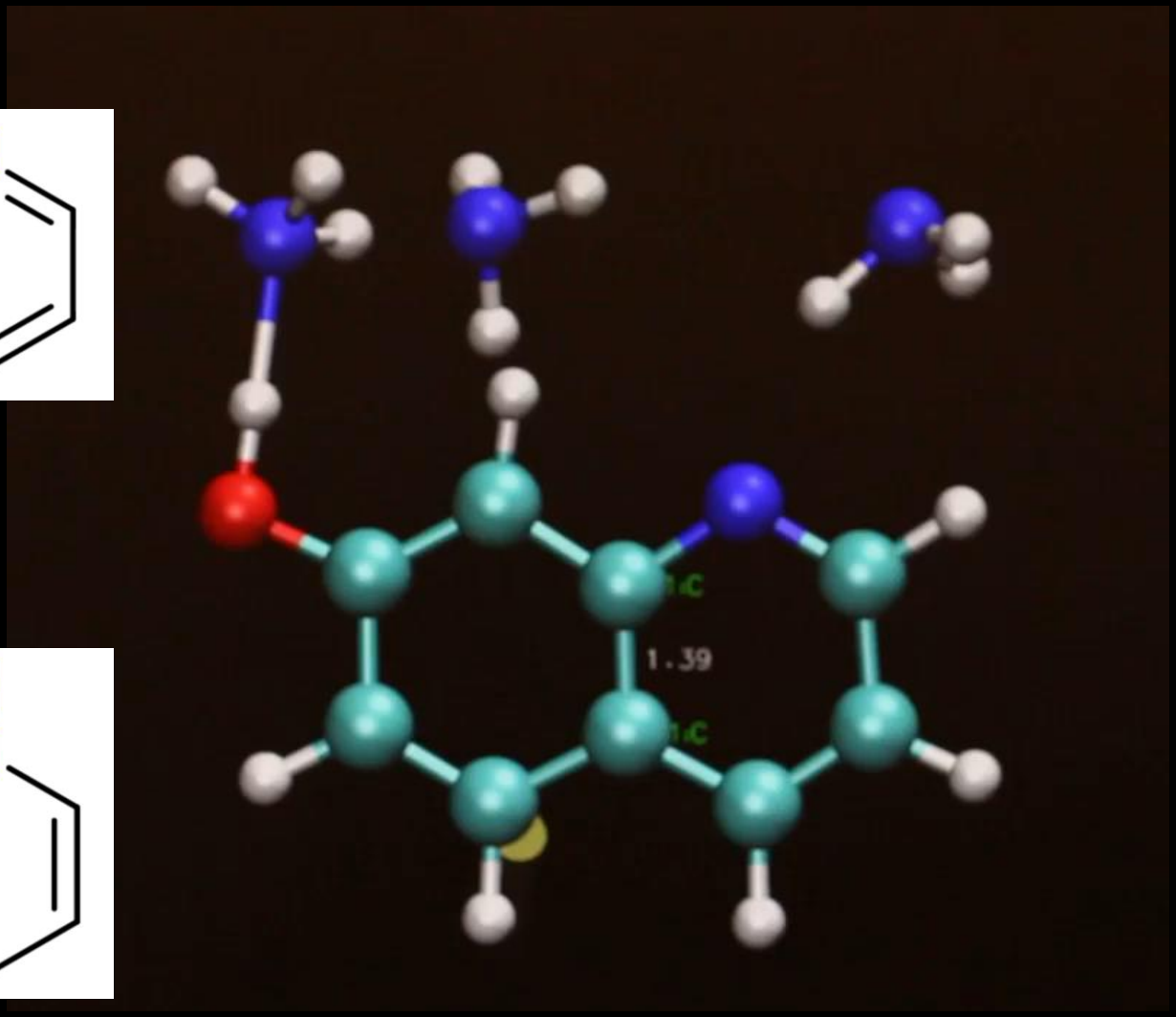


Ex3: Ammonia Wire

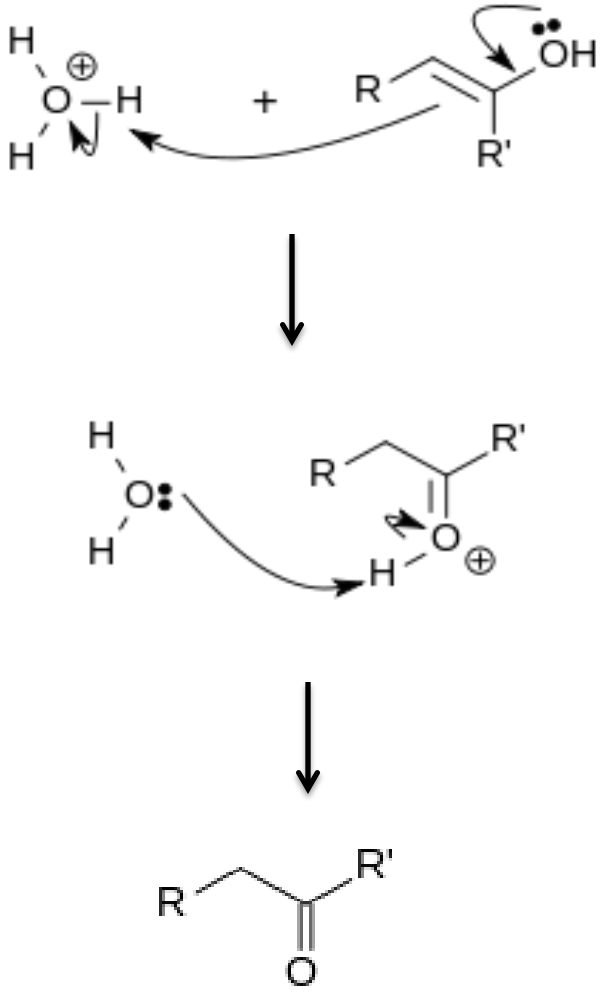


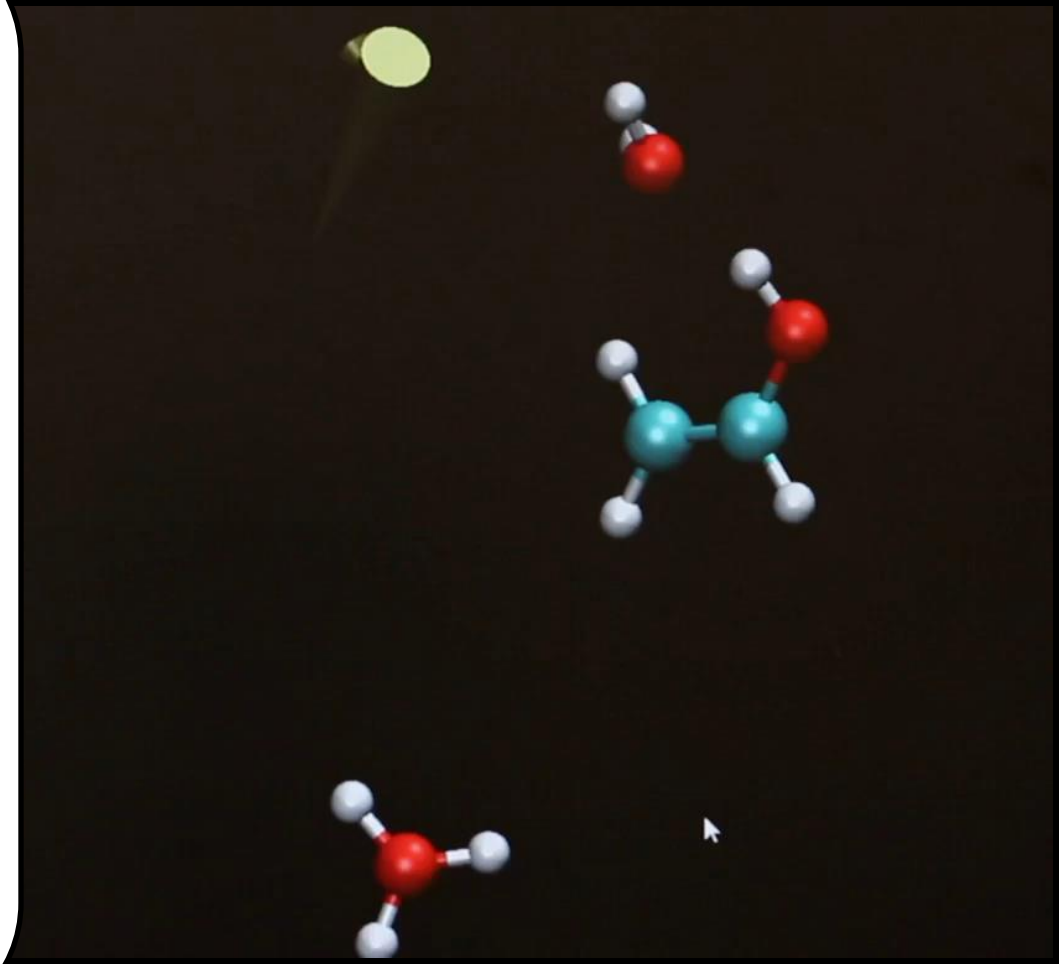
VS





Ex4: Keto-Enol Isomerization





Conclusions

- TeraChem running on GPUs enables interactive quantum chemistry for systems up to a few dozen atoms.

- Natural, tactile computer interfaces allow us to rapidly develop intuitive insight from simulations.

Acknowledgements

Martinez Group

Co-contributors:

- Alex Jin
- Alan Yee