# Massively-Parallel Real-Time TDDFT Modules for Non-Equilibrium Electron Dynamics

NSF: SI2-SSE project (Oct. 2017~)

Yi Yao, Alina Kononov, Erik Draeger (Collaborator), Andre Schleife (co-PI), Yosuke Kanai (lead-PI)

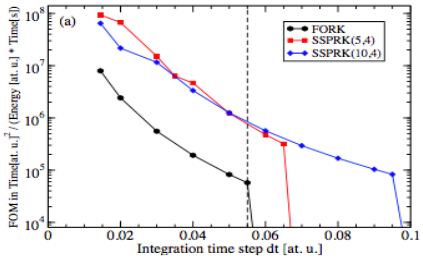
## Real-Time Time-Dependent Density Functional Theory (RT-TDDFT) Simulations

$$\left\{ i\hbar \frac{d}{dt} \left| \phi_i(t) \right\rangle = \hat{H}_{KS} \left| \phi_i(t) \right\rangle \right\}_{i=1..N} \qquad \hat{H}_{KS} \equiv -\frac{\hbar^2}{2m_e}\nabla^2 + \hat{V}_{ext}(t) + \hat{V}_H[\{\phi_i(t)\}] + \hat{V}_{XC}[\{\phi_i(t)\}]$$

**Coupled non-linear PDEs w/ millions of PWs for representing the single-particle states.** $\phi_i(\mathbf{r},t) = \psi_{n\mathbf{k}}(\mathbf{r},t) = \frac{1}{\sqrt{\Omega}} \sum_{\mathbf{G}}^{\mathbf{G}_{max}} C_n(\mathbf{G},\mathbf{k},t) e^{i(\mathbf{k}+\mathbf{G})\cdot\mathbf{r}}$

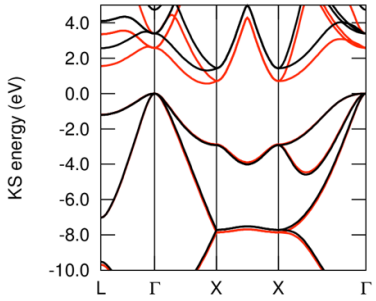
## Challenges addressed through development of new modules in Qb@ll code

### Highly scalable explicit integrators

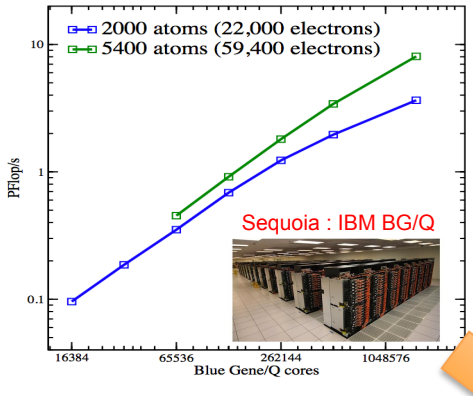



Recent *Strong Stability-Preserving Runge-Kutta (SSPRK)* methods to reduce "time-to-solution".

### Advanced and efficient approximation to $V_{xc}$




Recent *Strongly Constrained and Approximately Normed (SCAN)* approximation to improve accuracy at a reasonable increase in computational cost.




**HPC Software Infrastructure**

>40% peak performance
@ 1.6 million cores

- Massively parallel and tailored to modern HPCs with hybrid MPI/open-MP/SIMD.

**Scientific Impacts**

Simulating electronic excitation dynamics in solvated DNA under proton irradiation.

> 12,000 electrons
> 6,000,000 PWs
> 131,000 cores on BG/Q