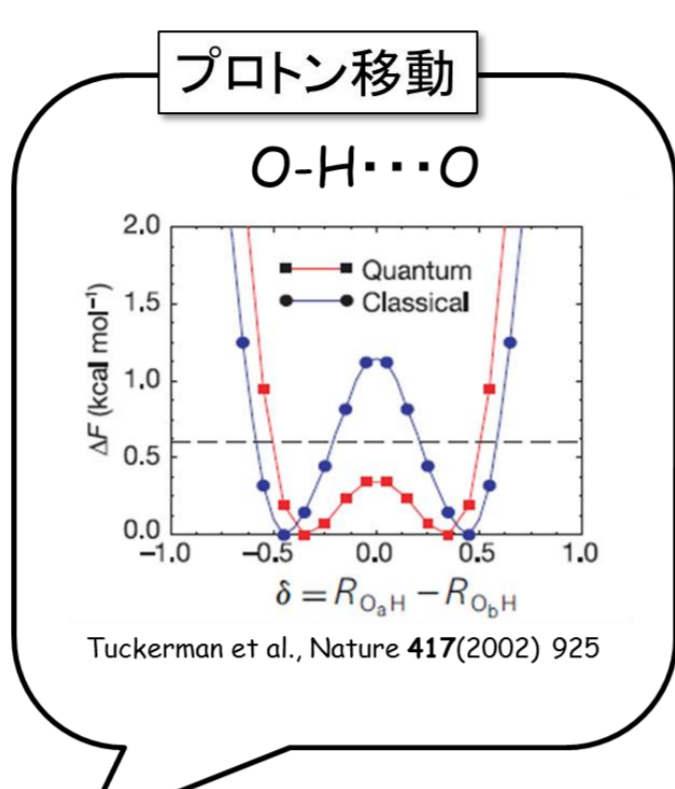
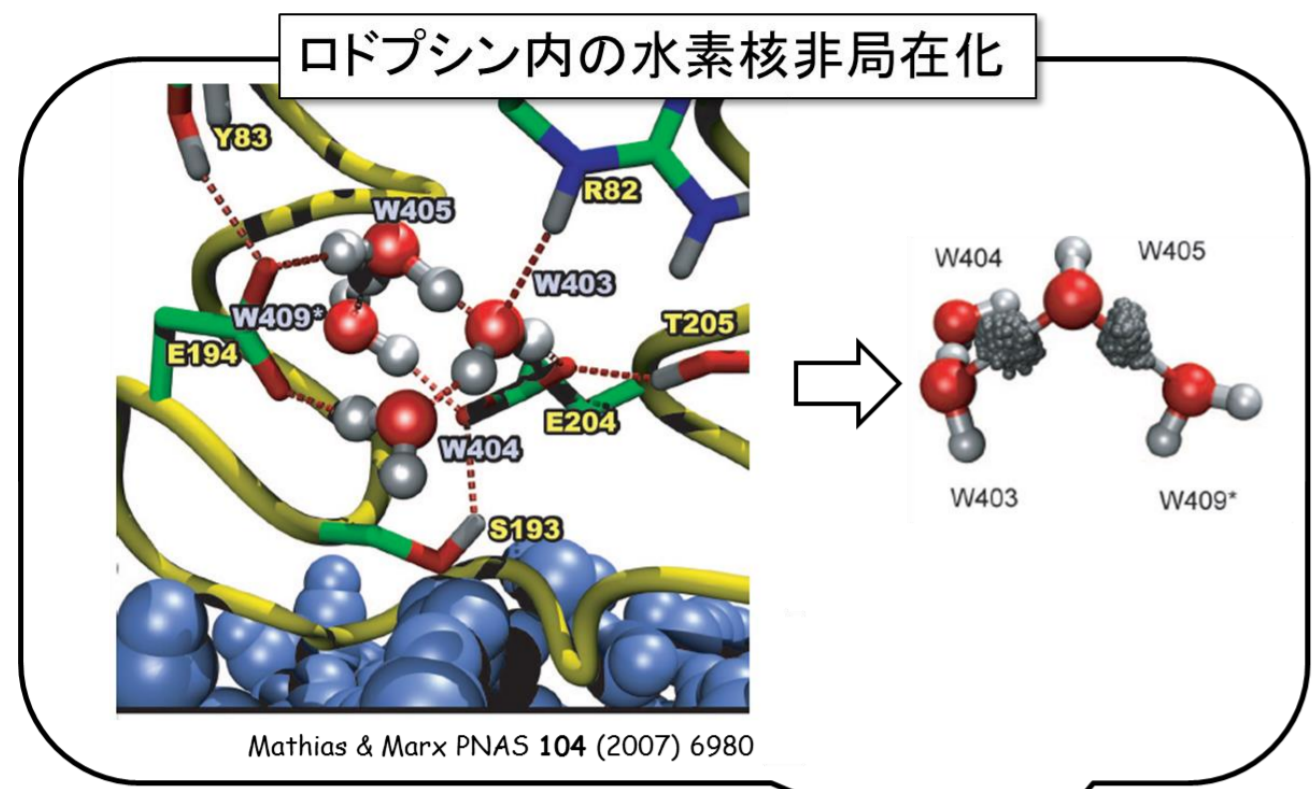
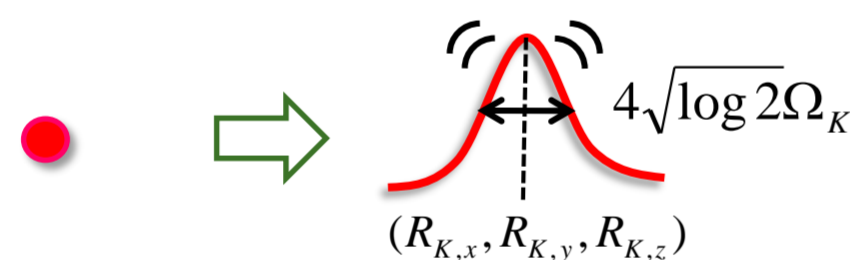
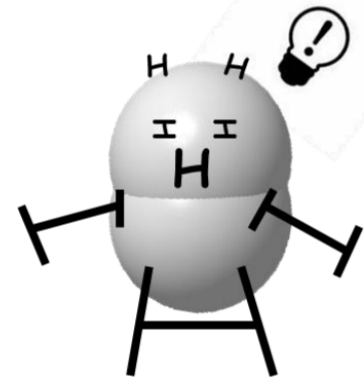
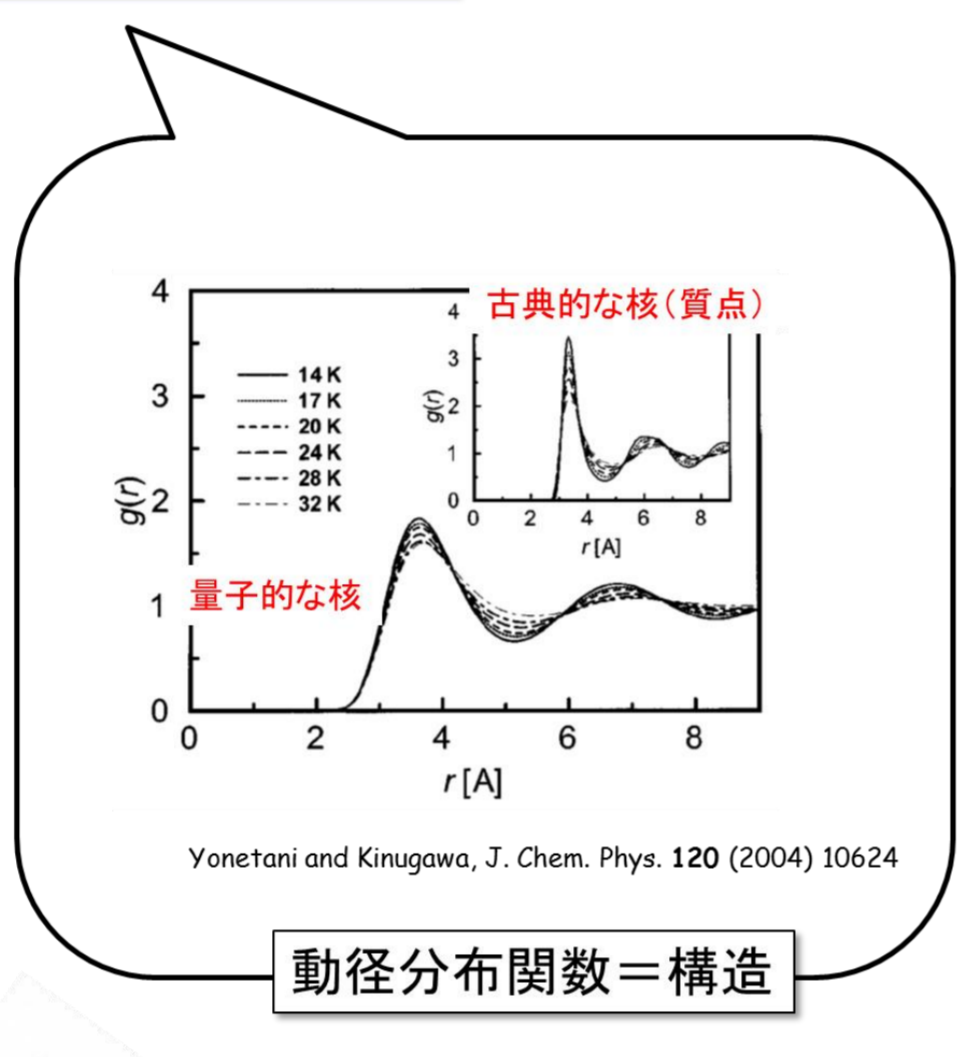
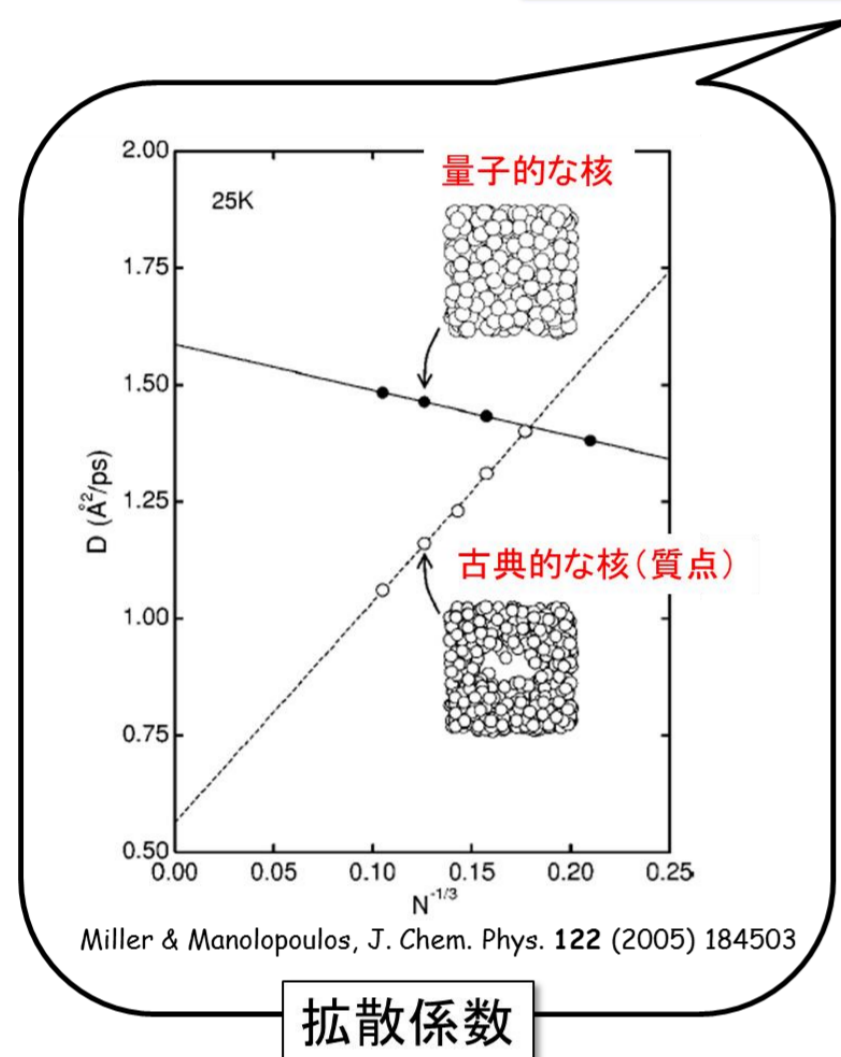


金賢得 (京都大学 大学院理学研究科)

# 水素の室温大量貯蔵・輸送を実現する多孔性材料の分子ダイナミクスに基づく解明と先導的デザイン



**水素が示す様々な核量子性**



**核量子効果**  
ゼロ点エネルギー  
核の非局在化

**量子分子動力学法**

**時間依存した二量体の波動関数**

$$\psi(t) = \mathcal{A}[\phi_a(\mathbf{q}_1)\phi_b(\mathbf{q}_2)\phi_c(\mathbf{q}_3)\phi_d(\mathbf{q}_4)\Theta(1,2,3,4)\Phi_A(\mathbf{Q}_1)\Phi_B(\mathbf{Q}_2)\Phi_C(\mathbf{Q}_3)\Phi_D(\mathbf{Q}_4)]$$

$\mathcal{A}$ : 反対称化オペレータ

Perfect-Pairing Valence Bond 理論: (a,b) (c,d) が Singlet

$$\Theta(1,2,3,4) = \frac{(\alpha(1)\beta(2) - \beta(1)\alpha(2))(\alpha(3)\beta(4) - \beta(3)\alpha(4))}{\sqrt{2}\sqrt{2}}$$

可変ガウス型波束

$$\Phi_K(\mathbf{Q}_i) \equiv \left(\frac{1}{2\pi\Omega_K^2(t)}\right)^{3/4} \exp\left[-\frac{(\mathbf{Q}_i - \mathbf{R}_K(t))^2}{4\Omega_K^2(t)} + \frac{i\Pi_K(t)}{2\Omega_K(t)}(\mathbf{Q}_i - \mathbf{R}_K(t))^2 + i\mathbf{P}_K(t) \cdot (\mathbf{Q}_i - \mathbf{R}_K(t))\right]$$

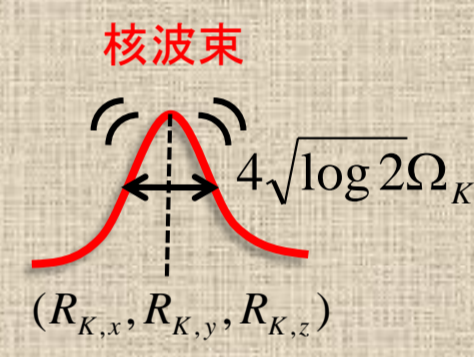
**時間依存変分原理**

作用積分  $\Gamma \equiv \int L dt = \int dt \langle \psi, t | i \frac{\partial}{\partial t} - \hat{H} | \psi, t \rangle$

ハミルトニアン  $\hat{H} = \sum_{i=1}^4 -\frac{1}{2M_{\text{nuc}}} \frac{\partial^2}{\partial Q_i^2} + V(\mathbf{q}_1, \mathbf{q}_2, \mathbf{q}_3, \mathbf{q}_4; \mathbf{Q}_1, \mathbf{Q}_2, \mathbf{Q}_3, \mathbf{Q}_4)$

**運動方程式**

$$\begin{aligned} \dot{\mathbf{R}}_K &= \frac{\partial H_{\text{ext}}}{\partial \mathbf{P}_K}, & \dot{\mathbf{P}}_K &= -\frac{\partial H_{\text{ext}}}{\partial \mathbf{R}_K}, \\ \dot{\Omega}_K &= \frac{1}{3} \frac{\partial H_{\text{ext}}}{\partial \Pi_K}, & \dot{\Pi}_K &= -\frac{1}{3} \frac{\partial H_{\text{ext}}}{\partial \Omega_K} \end{aligned}$$



$$H_{\text{ext}} \equiv \sum_K^{A,B,C,D} \left[ \frac{\mathbf{P}_K^2}{2M_{\text{nuc}}} + \frac{3\Pi_K^2}{2M_{\text{nuc}}} + \frac{3\hbar^2}{8M_{\text{nuc}}\Omega_K^2} \right] + \langle V_{\text{ke,elec}} \rangle + \langle V_{\text{ee}} \rangle + \langle V_{\text{nn}} \rangle + \langle V_{\text{ne}} \rangle$$

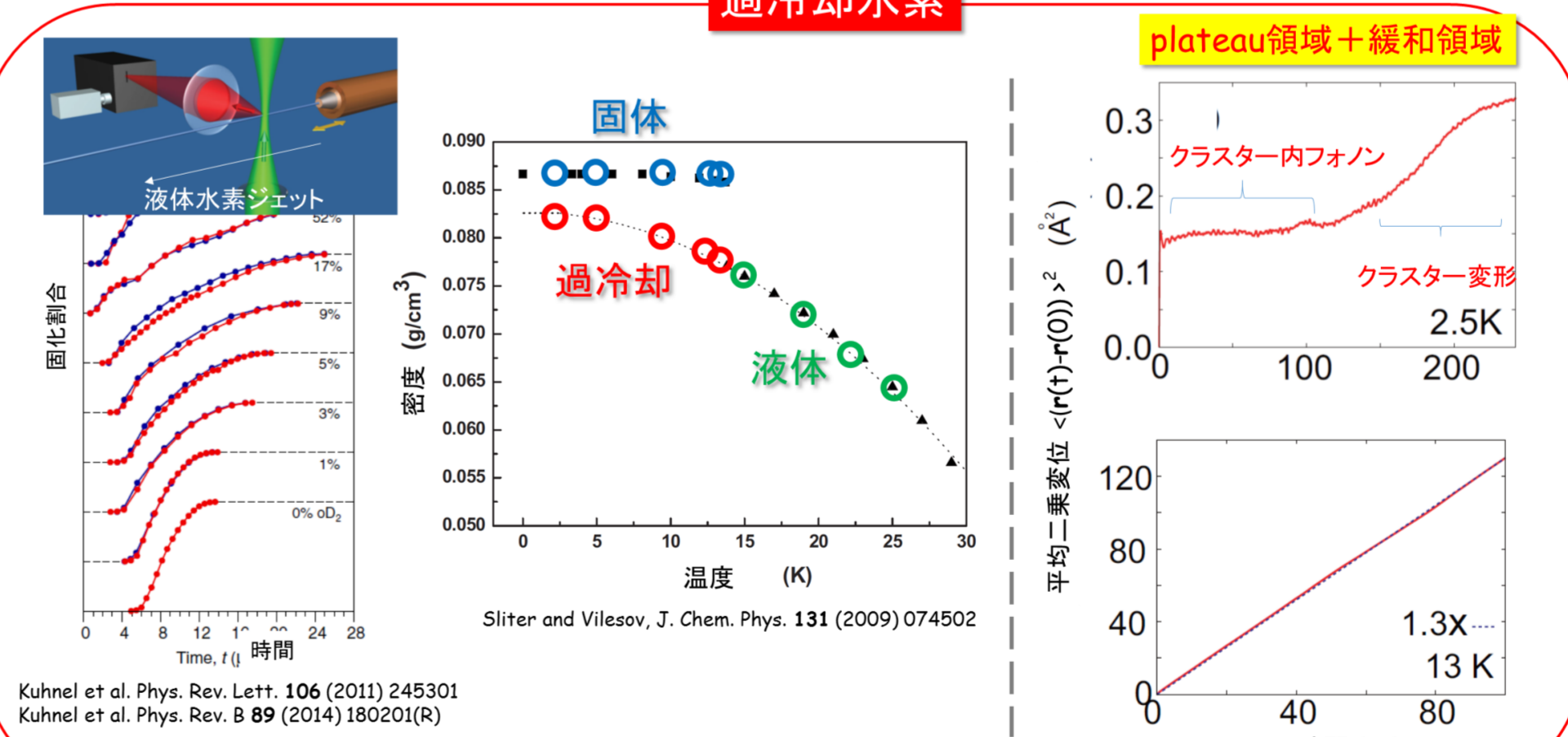
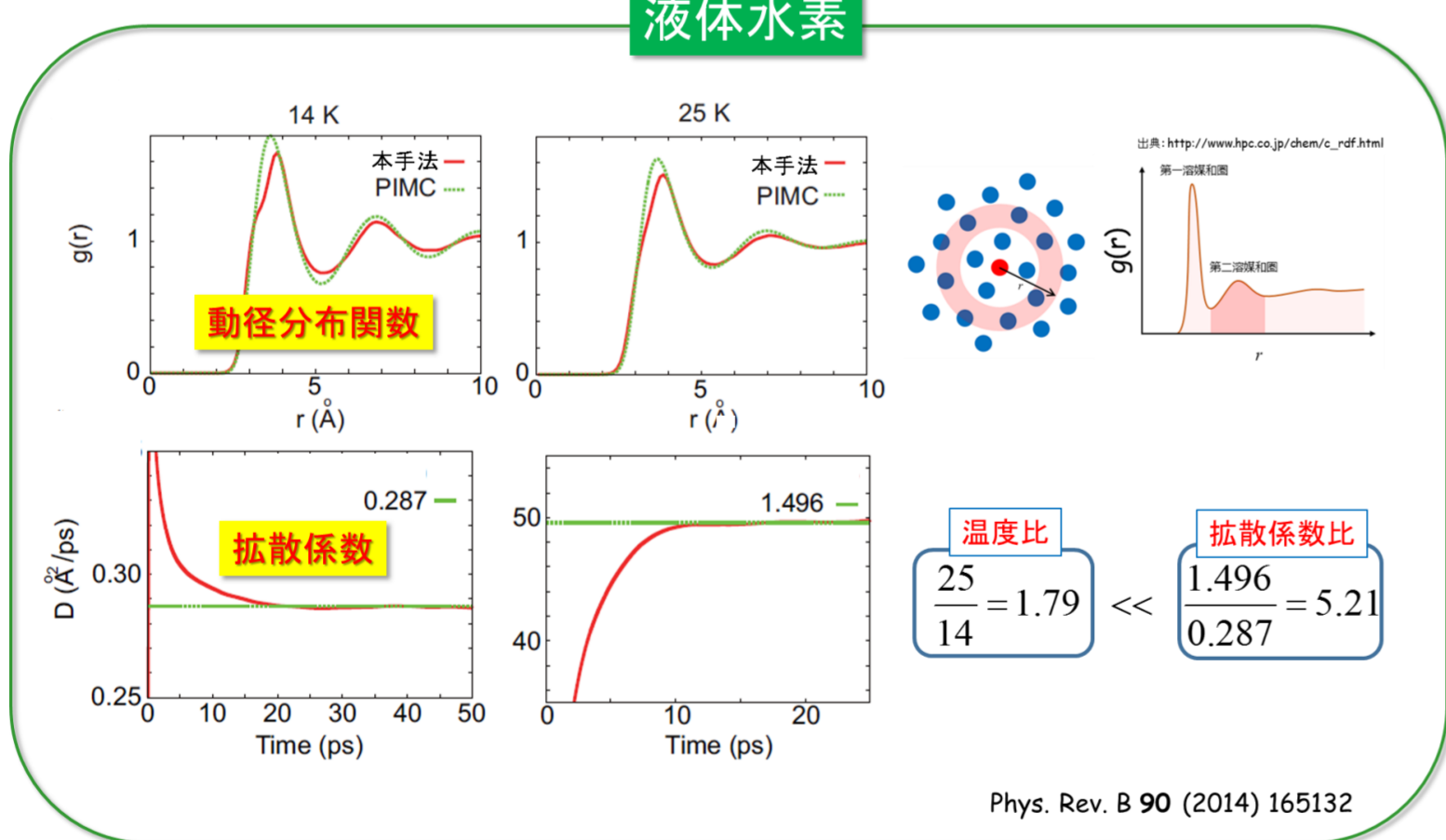
電子の運動エネルギー項      静電ポテンシャルエネルギー項

電子-電子  
核-核  
核-電子

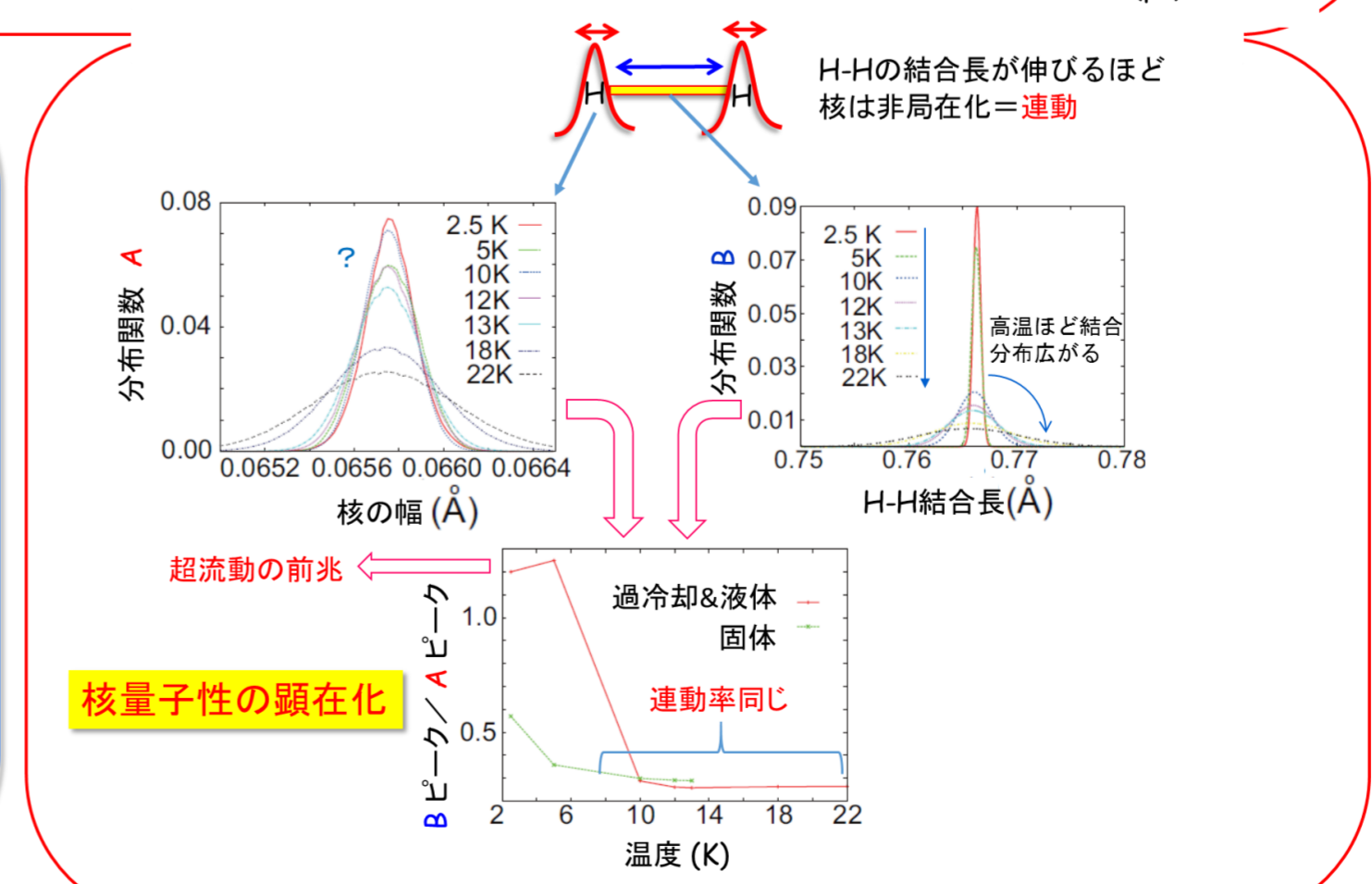
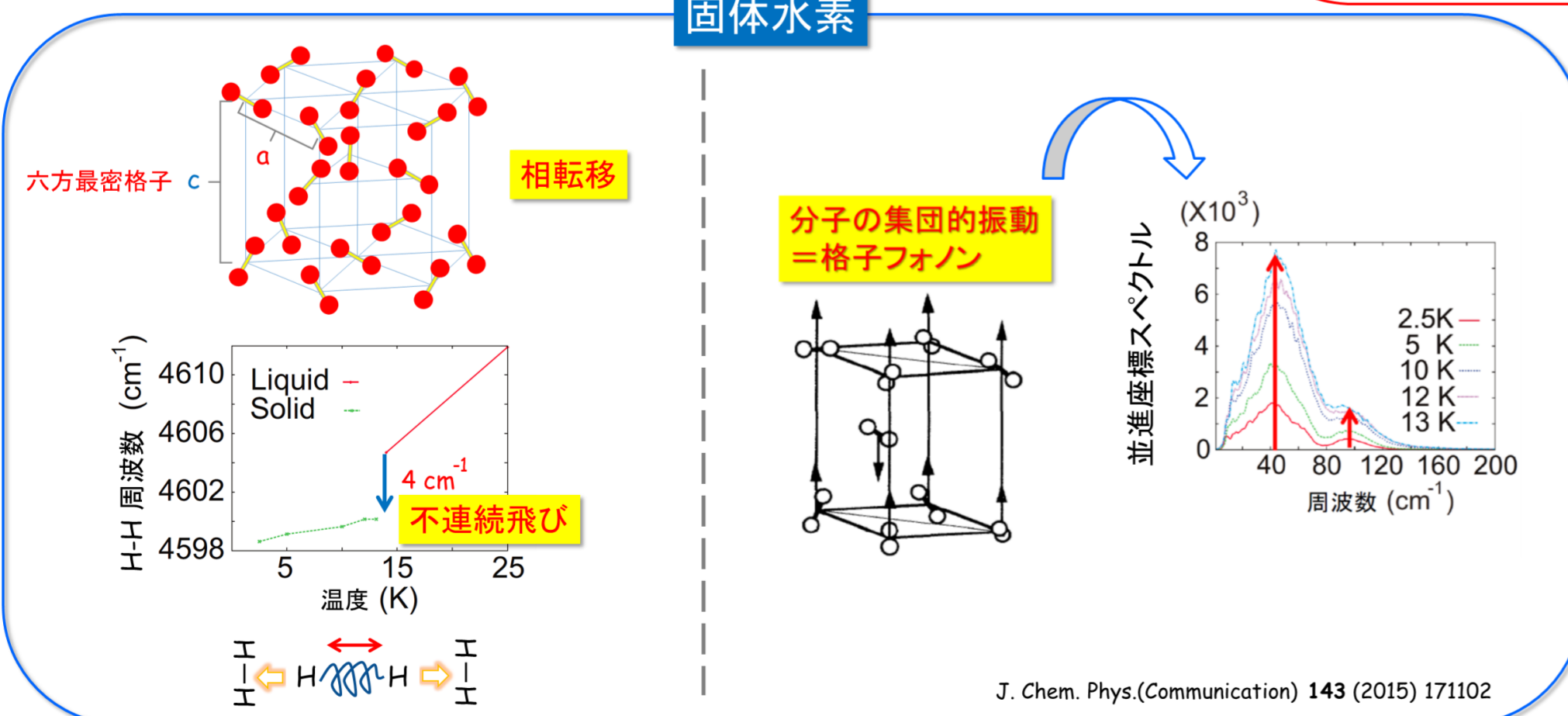
Chem. Phys. Lett. 532 (2012) 124  
J. Chem. Phys.(Communication) 140 (2014) 171101

足し合わせて多体系へ

**過冷却水素**



**固体水素**



\* 本研究課題の詳細は直接会場でお話いたします。