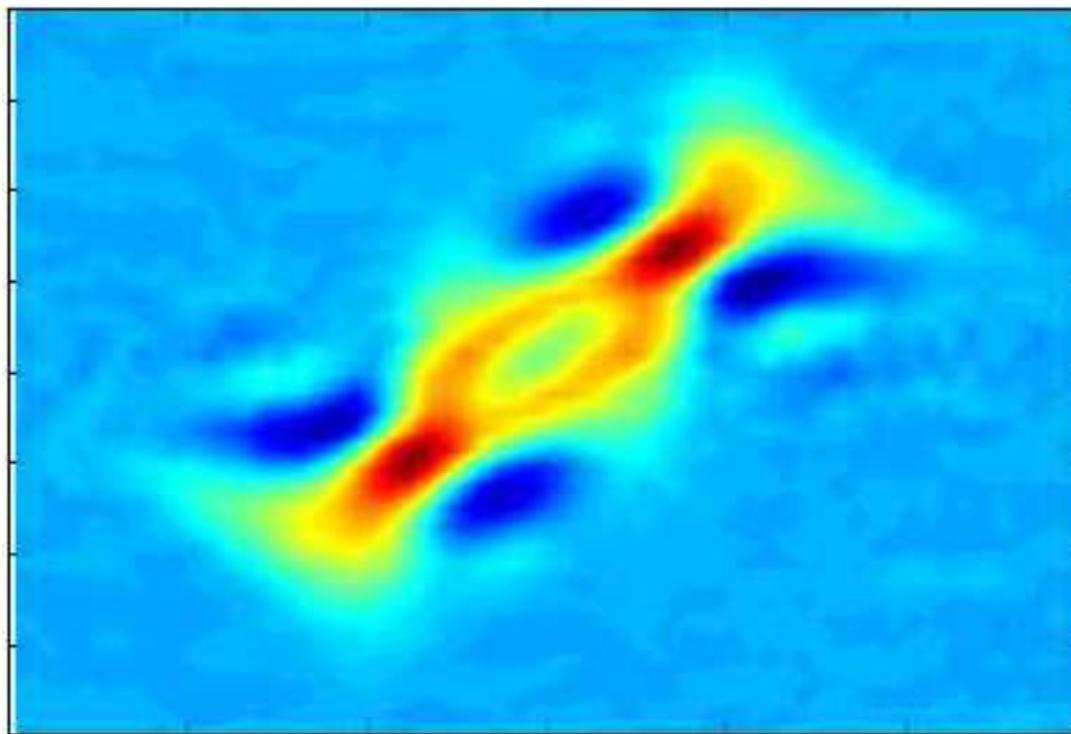
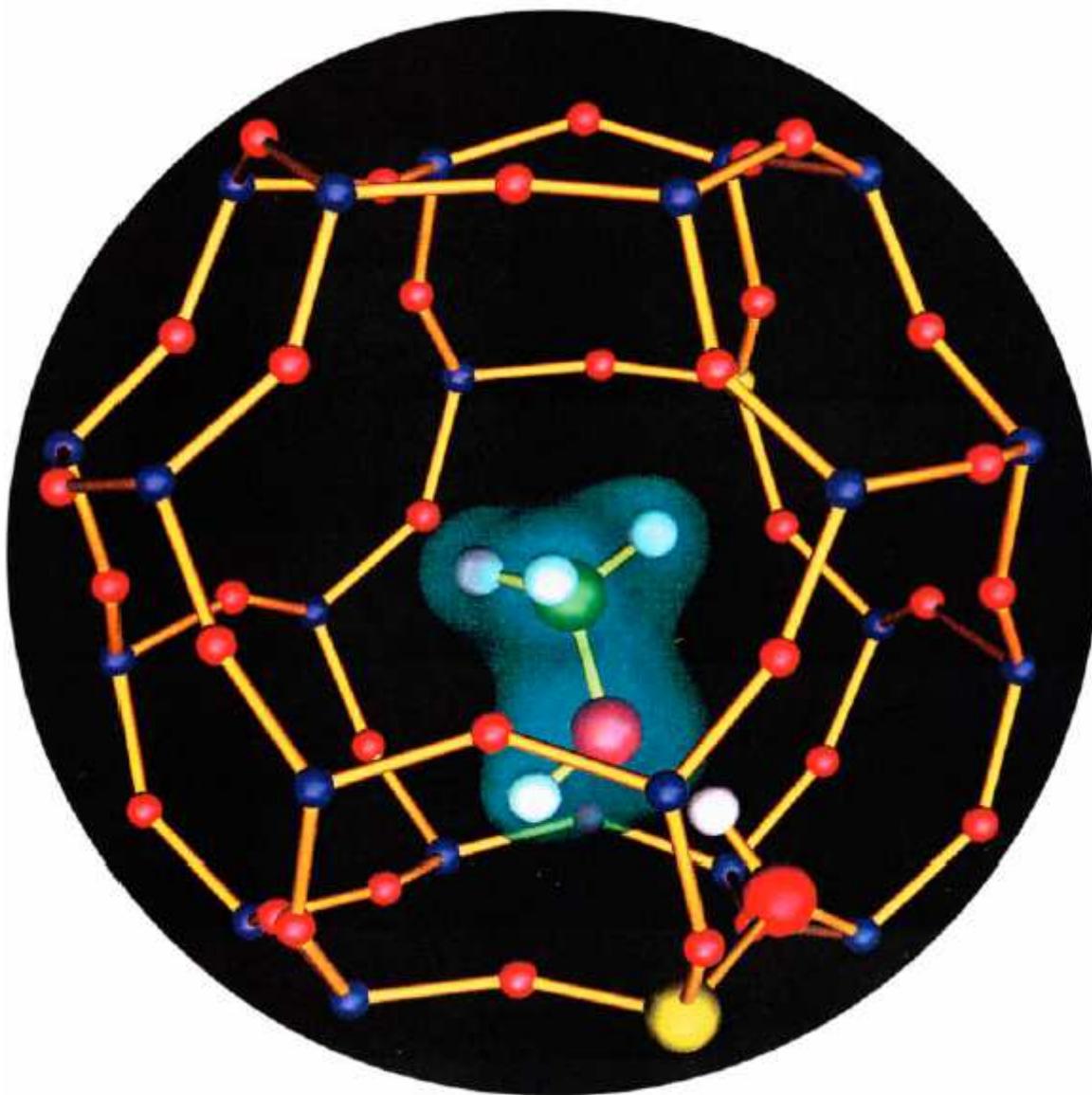


The Wigner Monte Carlo method for Density Functional Theory



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W. Kohn: Electronic structure of matter (Nobel Lecture)

PHYSICAL REVIEW

VOLUME 136, NUMBER 3B

9 NOVEMBER 1964

Inhomogeneous Electron Gas*

P. HOHENBERG†

École Normale Supérieure, Paris, France

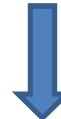
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(Received 18 June 1964)



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Self-Consistent Equations Including Exchange and Correlation Effects*

W. KOHN AND L. J. SHAM

University of California, San Diego, La Jolla, California

(Received 21 June 1965)



Density-Functional Theory for Time-Dependent Systems

Phys. Rev. Lett. **52**, 997 – Published 19 March 1984

Erich Runge and E. K. U. Gross

The Kohn-Sham system

$$i\hbar \frac{\partial \Phi_i}{\partial t} (\mathbf{r}, t) = \left(-\frac{\hbar^2 \nabla^2}{2m_i} + v_{\text{eff}}(\mathbf{r}) \right) \Phi_i(\mathbf{r}, t)$$

$$\rho(\mathbf{r}) = \sum_i |\Phi_i(\mathbf{r})|^2$$

$$(i = 1 \dots N)$$

Exchange-Correlation functional

$$v_{\text{eff}}(\mathbf{r}) = v_{\text{ext}}(\mathbf{r}) + e^2 \int d\mathbf{r}' \frac{\rho(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} + v_{\text{xc}}[\rho](\mathbf{r})$$

$$v_{\text{xc}}[\rho](\mathbf{r}) = -\frac{1}{\pi} [3\pi^2 \rho(\mathbf{r})]^{\frac{1}{3}}$$

Wigner-Weyl transform

$$\begin{aligned}\hat{A}(\hat{q}, \hat{p}) &\mapsto V_W(\hat{A}) = A(x, p) = \\ &= \frac{\hbar}{2\pi} \int d\xi \int d\eta \operatorname{Tr} \{ \hat{A}(\hat{q}, \hat{p}) e^{i\xi \hat{q} + i\eta \hat{p}} \} e^{-i\xi x - i\eta p}\end{aligned}$$

$$\left\{ \begin{array}{ll} A * B & \equiv V_W(\hat{A} \cdot \hat{B}) \\ [A, B]_M & \equiv \frac{1}{i\hbar} (A * B - B * A) \end{array} \right.$$

DFT in the Wigner formalism

$$\frac{\partial f_w^i}{\partial t} + \frac{\mathbf{p}}{m} \cdot \nabla_{\mathbf{r}} f_w^i = Q[f_w^i]$$

$$Q[f_w](\mathbf{r}, \mathbf{p}, t) = \int d\mathbf{p}' V_w(\mathbf{r}, \mathbf{p} - \mathbf{p}', t) f_w(\mathbf{r}, \mathbf{p}', t)$$

$$V_w(\mathbf{r}, \mathbf{p}, t) = \frac{1}{i\hbar^2(2\pi)^3} \int d\mathbf{r}' e^{-i\frac{\mathbf{p}\cdot\mathbf{r}'}{\hbar}} \left(v_{\text{eff}}\left(\mathbf{r} + \frac{\mathbf{r}'}{2}, t\right) - v_{\text{eff}}\left(\mathbf{r} - \frac{\mathbf{r}'}{2}, t\right) \right)$$

$$(i = 1 \dots N)$$

Applications

A Wigner Monte Carlo approach to density functional theory

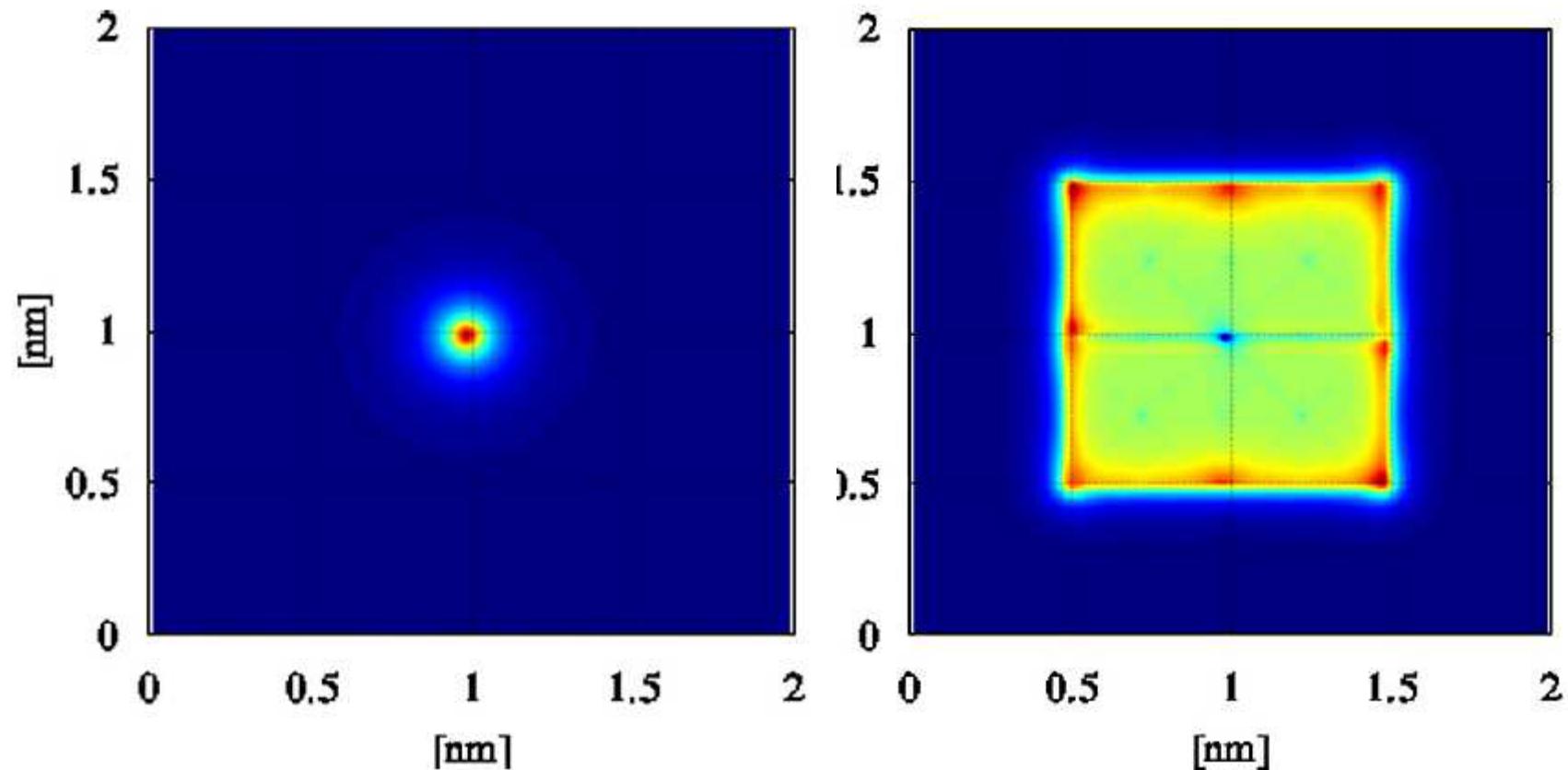
J.M. Sellier*, I. Dimov

Journal of Computational Physics 270 (2014) 265–277

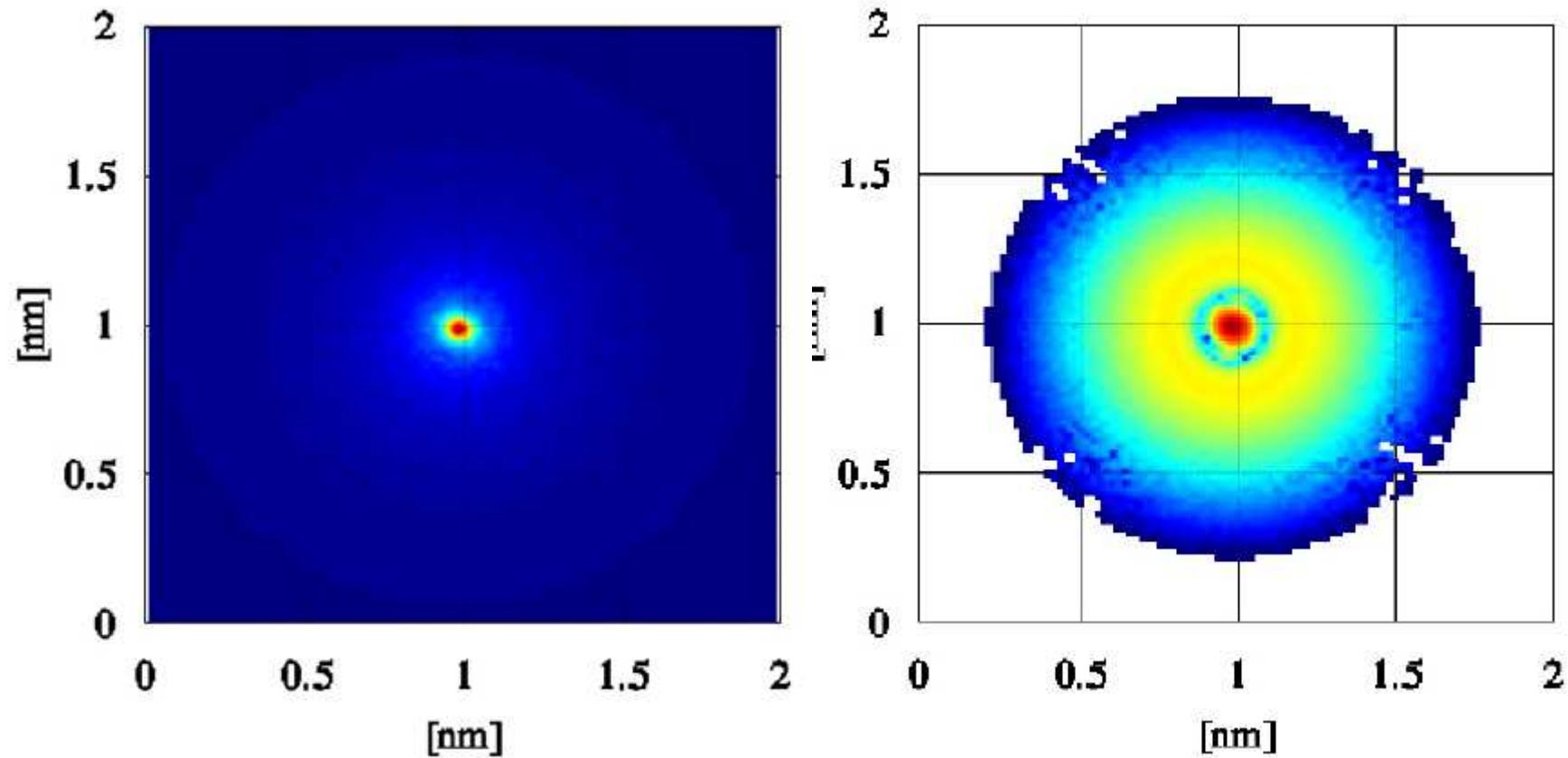
$$f_w^{1s}(\mathbf{r}, \mathbf{p}, 0) = A_{1s} e^{-\frac{-(\frac{p^2}{2m} - E_0)}{\sigma_E^2}} e^{-\frac{|\mathbf{r} - \mathbf{r}_i|}{a_0}}$$

$$f_w^{2s}(\mathbf{r}, \mathbf{p}, 0) = A_{2s} e^{-\frac{-(\frac{p^2}{2m} - E_0)}{\sigma_E^2}} e^{-\frac{|\mathbf{r} - \mathbf{r}_i|}{a_0}} \left(1 - \frac{|\mathbf{r} - \mathbf{r}_i|}{a_0}\right)$$

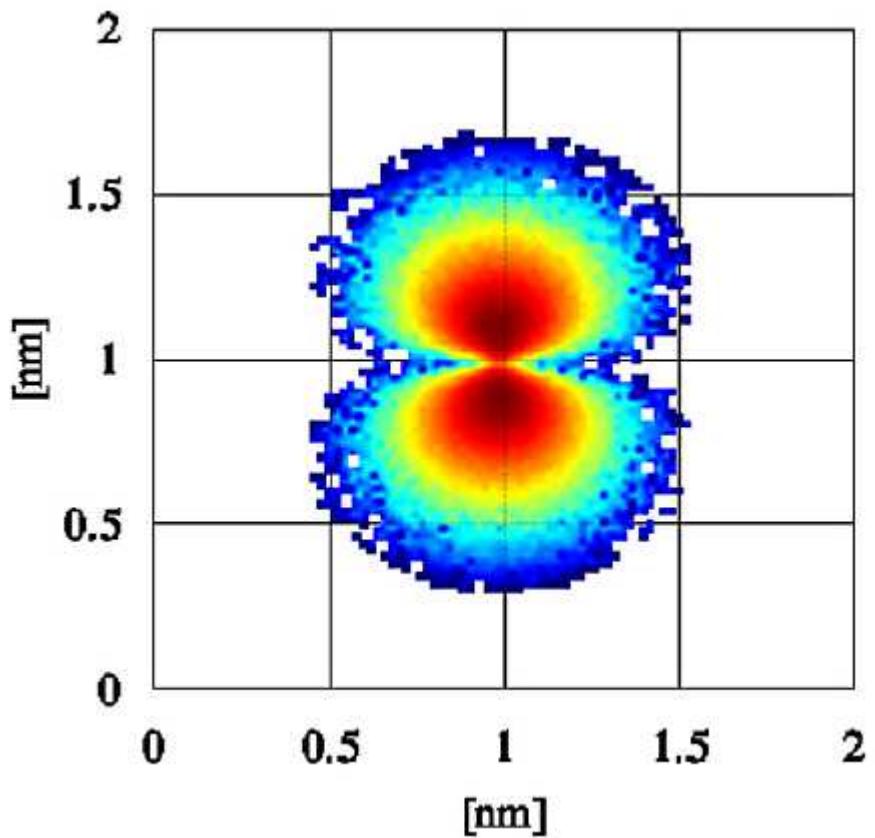
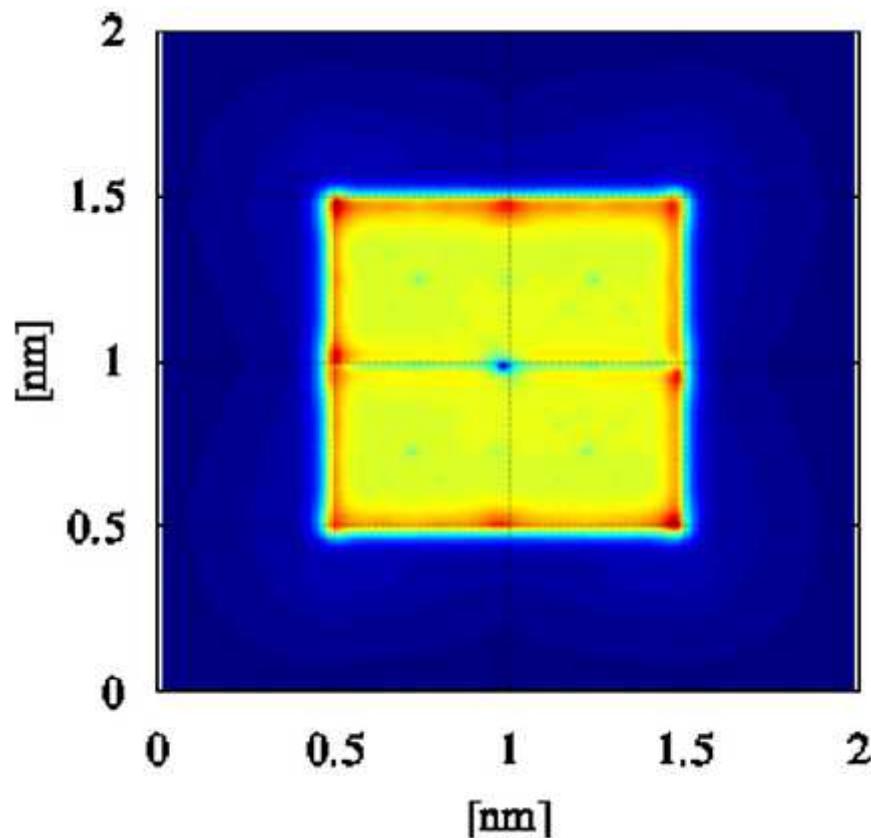
The lithium atom (3e⁻)



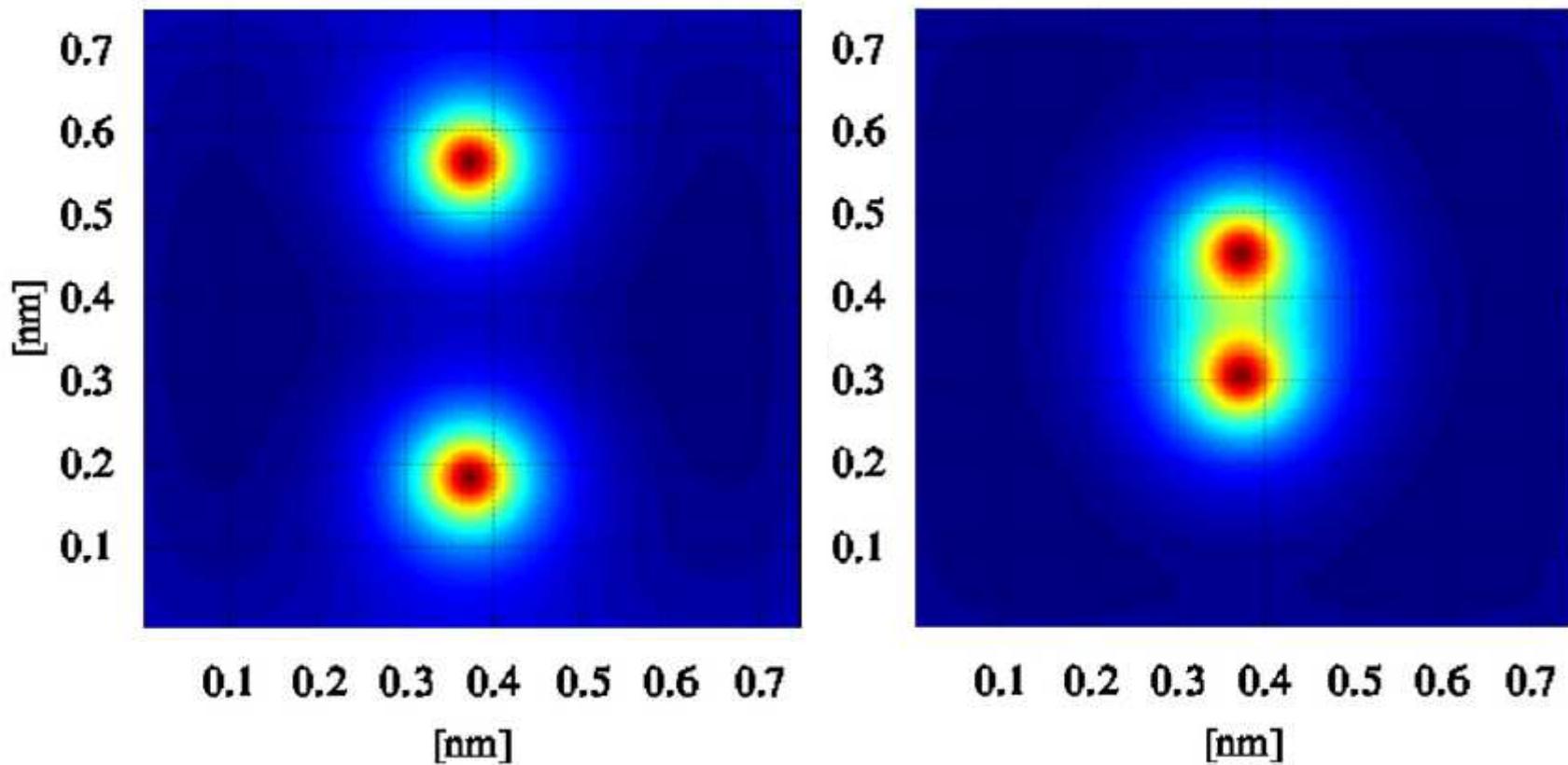
Lithium atom



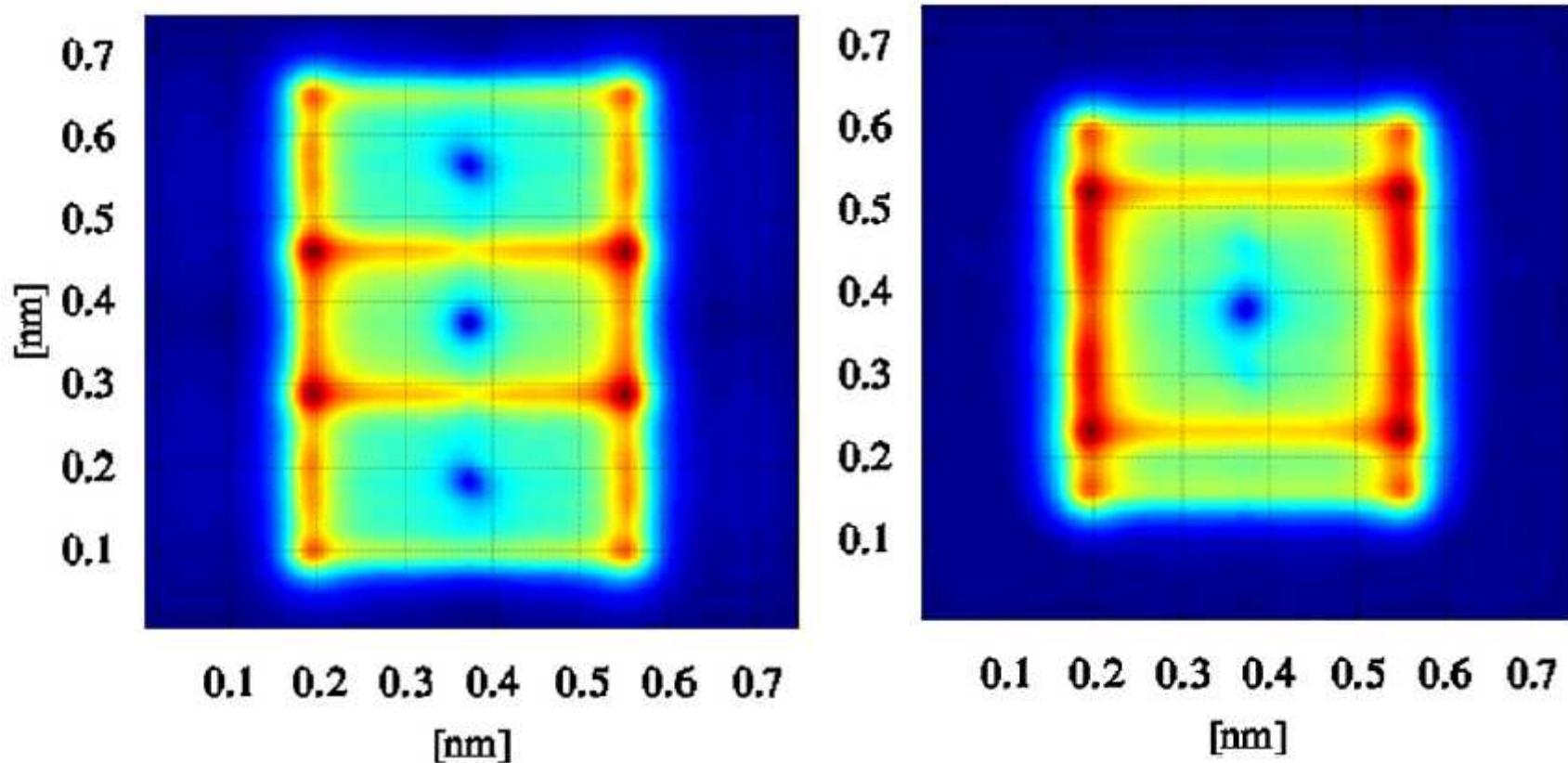
The boron atom (5e)



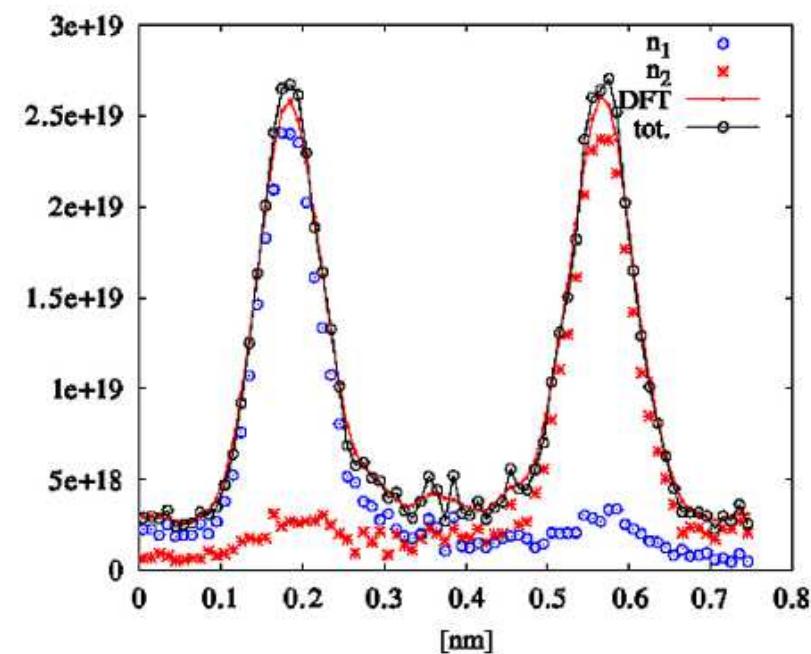
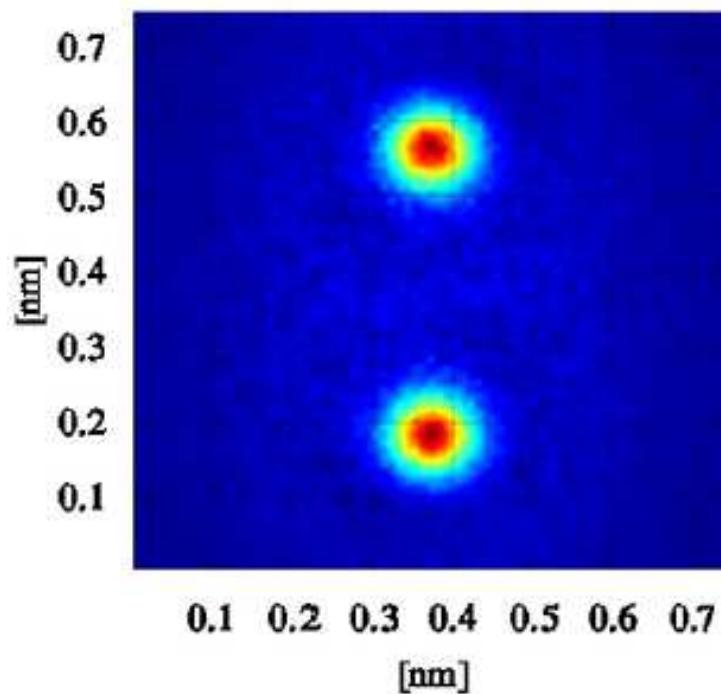
The H₂ molecule



The H₂ molecule



The H₂ molecule



The H_2 molecule

