

# シミュレーションで未来の 材料をデザインする

尾崎泰助  
HPCI戦略プログラム2  
東京大学物性研究所

# 元素の周期表

1 1IA 1A																	18 VIIIA 8A
1 <b>H</b> Hydrogen 1.0079	2 IIA 2A											13 IIIA 3A	14 IVA 4A	15 VA 5A	16 VIA 6A	17 VIIA 7A	2 <b>He</b> Helium 4.00260
3 <b>Li</b> Lithium 6.941	4 <b>Be</b> Beryllium 9.01218											5 <b>B</b> Boron 10.811	6 <b>C</b> Carbon 12.011	7 <b>N</b> Nitrogen 14.00674	8 <b>O</b> Oxygen 15.9994	9 <b>F</b> Fluorine 18.998403	10 <b>Ne</b> Neon 20.1797
11 <b>Na</b> Sodium 22.989768	12 <b>Mg</b> Magnesium 24.305	3 IIIB 3B	4 IVB 4B	5 VB 5B	6 VIB 6B	7 VIIB 7B	8 VIII 8	9 VIII 8	10 VIII 8	11 IB 1B	12 IIB 2B	13 <b>Al</b> Aluminum 26.981539	14 <b>Si</b> Silicon 28.0855	15 <b>P</b> Phosphorus 30.973762	16 <b>S</b> Sulfur 32.066	17 <b>Cl</b> Chlorine 35.4527	18 <b>Ar</b> Argon 39.948
19 <b>K</b> Potassium 39.0983	20 <b>Ca</b> Calcium 40.078	21 <b>Sc</b> Scandium 44.95591	22 <b>Ti</b> Titanium 47.88	23 <b>V</b> Vanadium 50.9415	24 <b>Cr</b> Chromium 51.9961	25 <b>Mn</b> Manganese 54.938	26 <b>Fe</b> Iron 55.847	27 <b>Co</b> Cobalt 58.9332	28 <b>Ni</b> Nickel 58.6934	29 <b>Cu</b> Copper 63.546	30 <b>Zn</b> Zinc 65.39	31 <b>Ga</b> Gallium 69.732	32 <b>Ge</b> Germanium 72.64	33 <b>As</b> Arsenic 74.92159	34 <b>Se</b> Selenium 78.96	35 <b>Br</b> Bromine 79.904	36 <b>Kr</b> Krypton 83.80
37 <b>Rb</b> Rubidium 85.4678	38 <b>Sr</b> Strontium 87.62	39 <b>Y</b> Yttrium 88.90585	40 <b>Zr</b> Zirconium 91.224	41 <b>Nb</b> Niobium 92.90638	42 <b>Mo</b> Molybdenum 95.94	43 <b>Tc</b> Technetium 98.9072	44 <b>Ru</b> Ruthenium 101.07	45 <b>Rh</b> Rhodium 102.9055	46 <b>Pd</b> Palladium 106.42	47 <b>Ag</b> Silver 107.8682	48 <b>Cd</b> Cadmium 112.411	49 <b>In</b> Indium 114.818	50 <b>Sn</b> Tin 118.71	51 <b>Sb</b> Antimony 121.760	52 <b>Te</b> Tellurium 127.6	53 <b>I</b> Iodine 126.90447	54 <b>Xe</b> Xenon 131.29
55 <b>Cs</b> Cesium 132.90543	56 <b>Ba</b> Barium 137.327	57-71	72 <b>Hf</b> Hafnium 178.49	73 <b>Ta</b> Tantalum 180.9479	74 <b>W</b> Tungsten 183.85	75 <b>Re</b> Rhenium 186.207	76 <b>Os</b> Osmium 190.23	77 <b>Ir</b> Iridium 192.22	78 <b>Pt</b> Platinum 195.08	79 <b>Au</b> Gold 196.9665	80 <b>Hg</b> Mercury 200.59	81 <b>Tl</b> Thallium 204.3833	82 <b>Pb</b> Lead 207.2	83 <b>Bi</b> Bismuth 208.98037	84 <b>Po</b> Polonium [208.9824]	85 <b>At</b> Astatine 209.9871	86 <b>Rn</b> Radon 222.0176
87 <b>Fr</b> Francium 223.0197	88 <b>Ra</b> Radium 226.0254	89-103	104 <b>Rf</b> Rutherfordium [261]	105 <b>Db</b> Dubnium [262]	106 <b>Sg</b> Seaborgium [266]	107 <b>Bh</b> Bohrium [264]	108 <b>Hs</b> Hassium [269]	109 <b>Mt</b> Meitnerium [268]	110 <b>Ds</b> Darmstadtium [269]	111 <b>Rg</b> Roentgenium [272]	112 <b>Cn</b> Copernicium [277]	113 <b>Uut</b> Ununtrium unknown	114 <b>Uuq</b> Ununquadium [289]	115 <b>Uup</b> Ununpentium unknown	116 <b>Uuh</b> Ununhexium [288]	117 <b>Uus</b> Ununseptium unknown	118 <b>Uuo</b> Ununoctium unknown
Lanthanide Series		57 <b>La</b> Lanthanum 138.9055	58 <b>Ce</b> Cerium 140.115	59 <b>Pr</b> Praseodymium 140.90765	60 <b>Nd</b> Neodymium 144.24	61 <b>Pm</b> Promethium 144.9127	62 <b>Sm</b> Samarium 150.36	63 <b>Eu</b> Europium 151.9655	64 <b>Gd</b> Gadolinium 157.25	65 <b>Tb</b> Terbium 158.92534	66 <b>Dy</b> Dysprosium 162.50	67 <b>Ho</b> Holmium 164.93032	68 <b>Er</b> Erbium 167.26	69 <b>Tm</b> Thulium 168.93421	70 <b>Yb</b> Ytterbium 173.04	71 <b>Lu</b> Lutetium 174.967	
Actinide Series		89 <b>Ac</b> Actinium 227.0278	90 <b>Th</b> Thorium 232.0381	91 <b>Pa</b> Protactinium 231.03588	92 <b>U</b> Uranium 238.0289	93 <b>Np</b> Neptunium 237.0482	94 <b>Pu</b> Plutonium 244.0642	95 <b>Am</b> Americium 243.0614	96 <b>Cm</b> Curium 247.0703	97 <b>Bk</b> Berkelium 247.0703	98 <b>Cf</b> Californium 251.0796	99 <b>Es</b> Einsteinium [254]	100 <b>Fm</b> Fermium 257.0951	101 <b>Md</b> Mendelevium 258.1	102 <b>No</b> Nobelium 259.1009	103 <b>Lr</b> Lawrencium [262]	
	Alkali Metal	Alkaline Earth	Transition Metal	Basic Metal	Semimetals	Nonmetals	Halogens	Noble Gas	Lanthanides	Actinides							

H<sub>2</sub>O



H<sub>2</sub>O

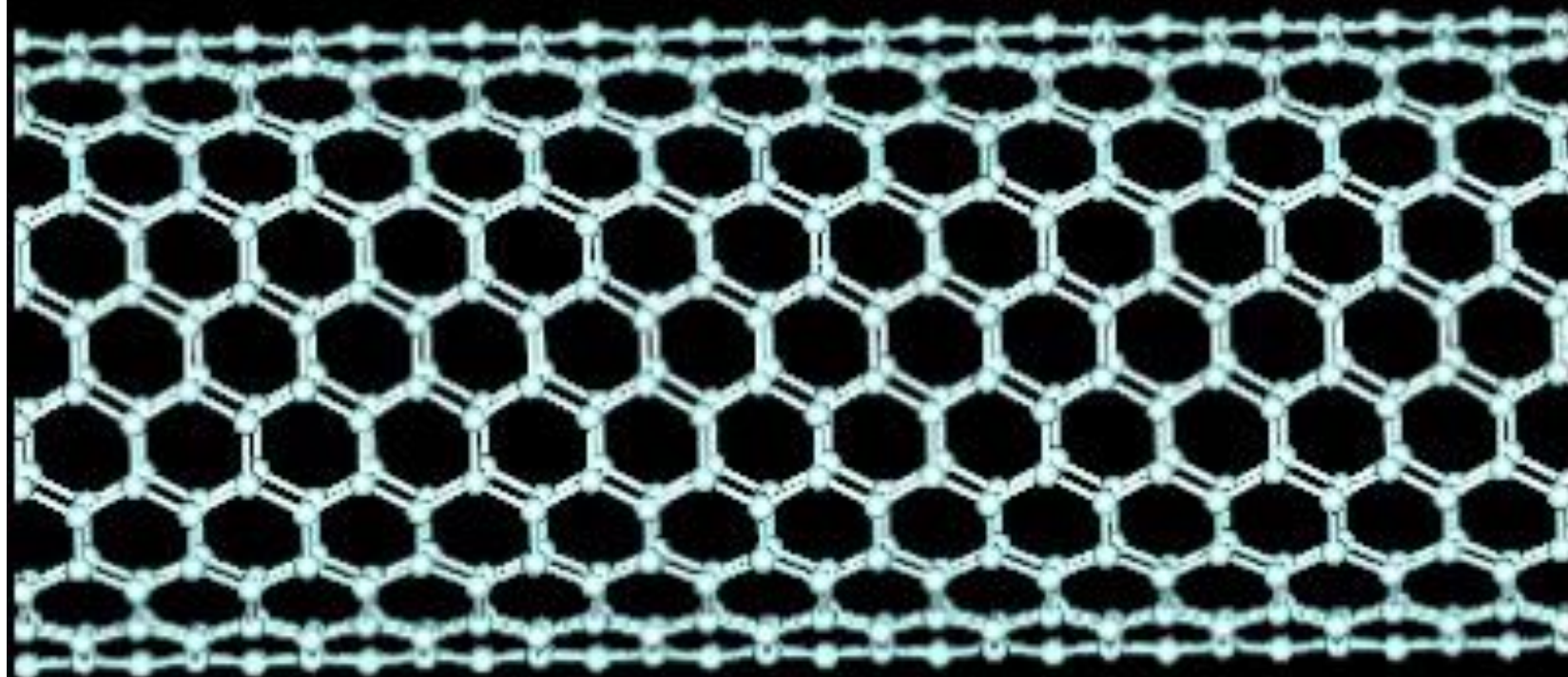




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Alkali Metal		Alkaline Earth		Transition Metal		Basic Metal		Semimetals		Nonmetals		Halogens		Noble Gas		Lanthanides		Actinides	

Frame #. 1

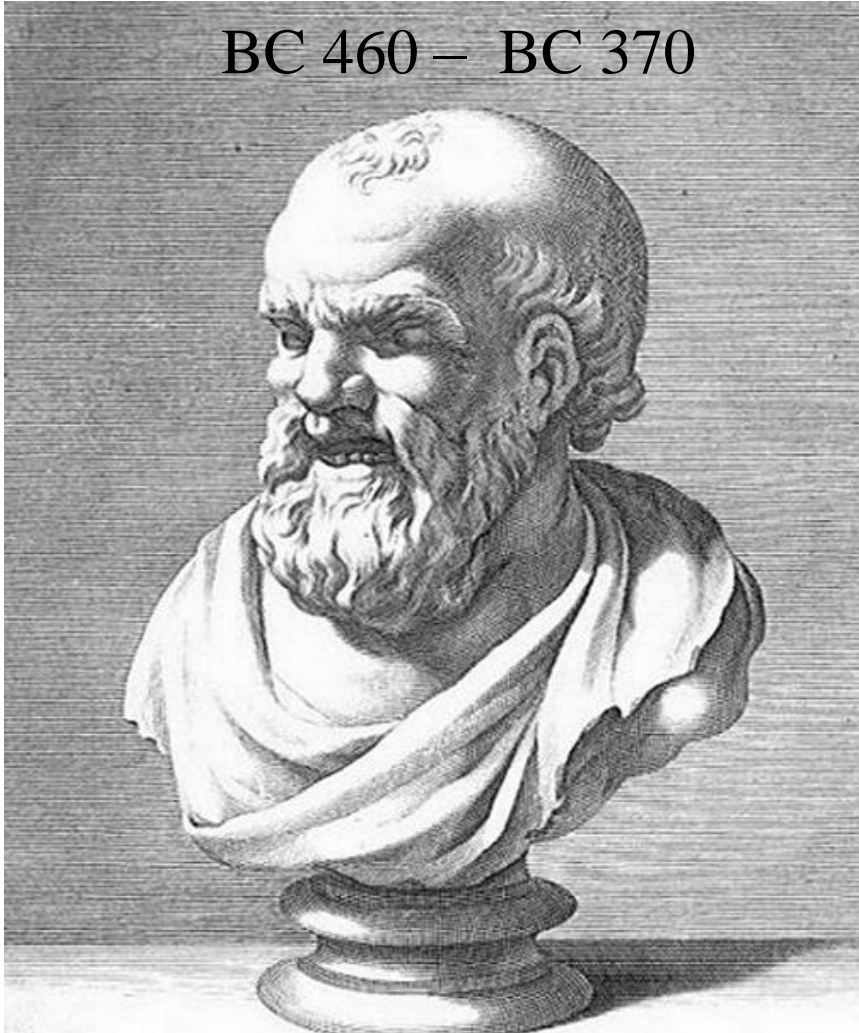




# デモクリトスの原子論

Democritus

BC 460 – BC 370



全てのものは原子でできている。原子はそれ以上、分割できない基本単位である。

# シュレディンガー方程式

$$i\hbar \frac{\partial}{\partial t} \Psi = \hat{H} \Psi$$

運動エネルギー      外部ポテンシャル      電子間相互作用

$$\hat{H} = -\frac{1}{2} \sum_{i=1}^{N_e} \left( \frac{\partial^2}{\partial x_i^2} + \frac{\partial^2}{\partial y_i^2} + \frac{\partial^2}{\partial z_i^2} \right) + \sum_i \sum_k \frac{Z_k}{|\mathbf{R}_k - \mathbf{r}_i|} + \sum_i \sum_{j>i} \frac{1}{|\mathbf{r}_i - \mathbf{r}_j|}$$



# コンピュータに解き方を教える!

```
double Calc_Ekin()
{
  /******
   calculate the kinetic energy, Ekin
  *****/

  int i, j, spin;
  int Mc_AN, Gc_AN, Cwan, Rn, h_AN, Gh_AN, Hwan;
  double My_Ekin, Ekin, Zc, Zh, dum, dum2;
  int numprocs, myid;
  double Stime_atom, Etime_atom;
  double *My_Ekin_threads;
  /* for OpenMP */
  int OMPID, Nthrds, Nthrds0, Nprocs, Nloop;

  /* MPI */
  MPI_Comm_size(MPI_COMM_WORLD, &numprocs);
  MPI_Comm_rank(MPI_COMM_WORLD, &myid);

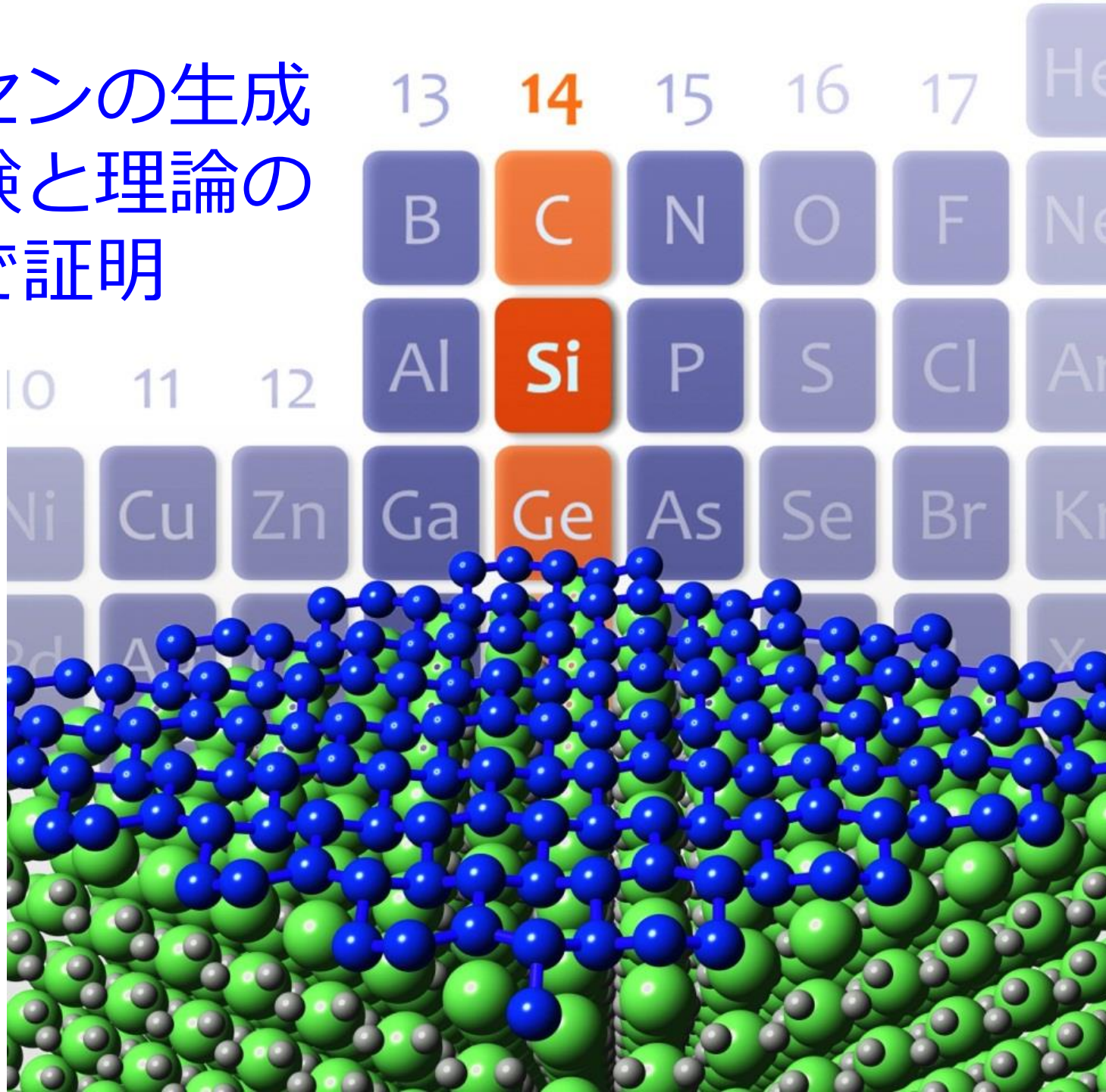
  /* get Nthrds0 */
  #pragma omp parallel shared(Nthrds0)
  {
    Nthrds0 = omp_get_num_threads();
  }

  /* allocation of array */
  My_Ekin_threads = (double*) malloc(sizeof(double)*Nthrds0);
  for (Nloop=0; Nloop<Nthrds0; Nloop++) My_Ekin_threads[Nloop] = 0.0;

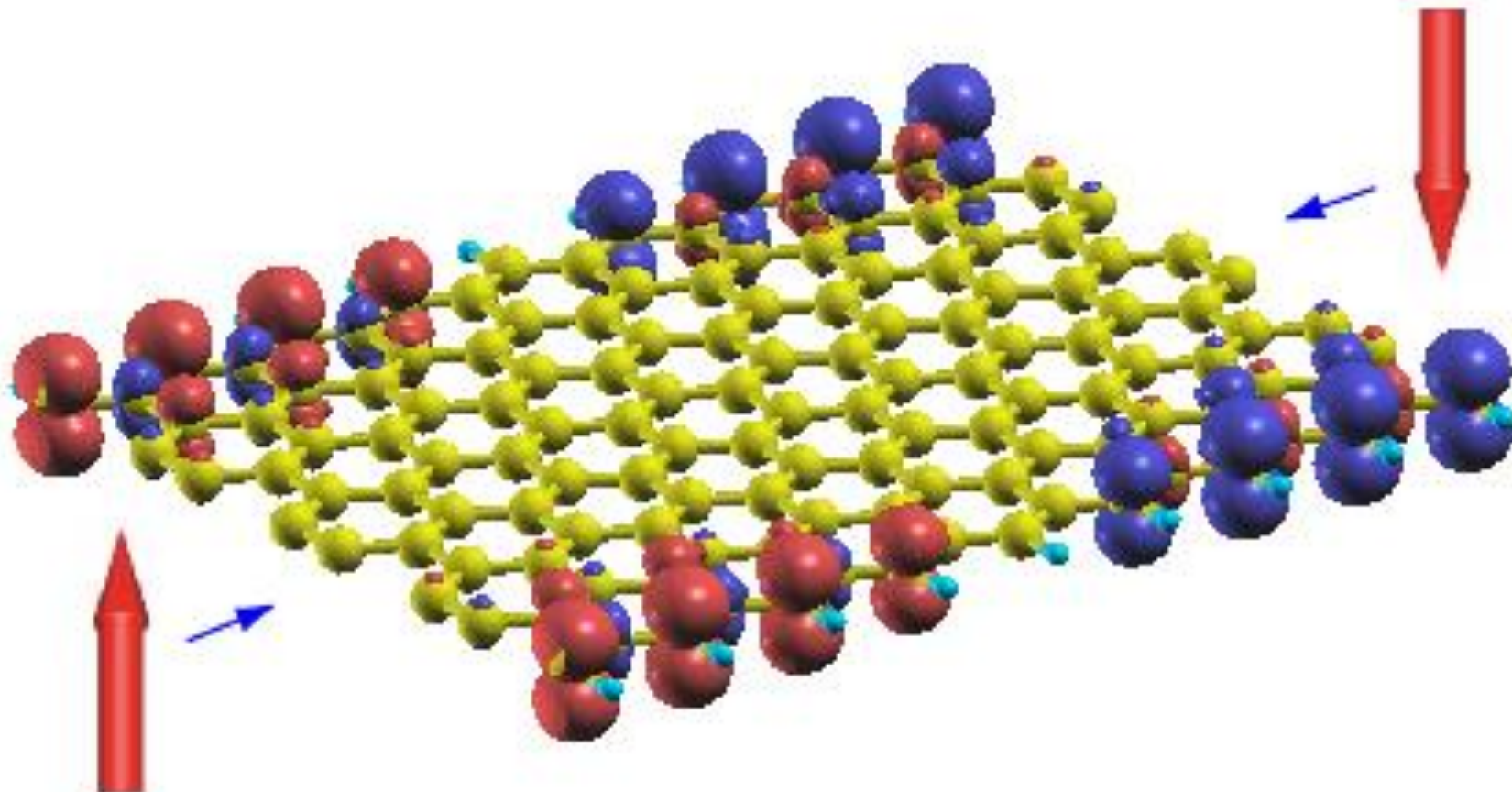
  if (SpinP_switch==0 || SpinP_switch==1) {
    for (spin=0; spin<=SpinP_switch; spin++) {
      #pragma omp parallel shared(SpinP_switch, time_per_atom, spin, CntH0, H0, DM, My_Ekin_threads, Spe_Total_CNO, Cnt_switch, natn\
, WhatSpecies, M2G, OneD2h_AN, OneD2Mc_AN, OneD_Nloop) private(OMPID, Nthrds, Nprocs, Nloop, Stime_atom, Mc_AN, h_AN, Gc_AN, Cwan, \
Gh_AN, Hwan, i, j, Etime_atom)
      {
        /* get info. on OpenMP */

        OMPID = omp_get_thread_num();
        Nthrds = omp_get_num_threads();
        Nprocs = omp_get_num_procs();
```

# シリセンの生成 を実験と理論の 連携で証明



# グラフェンナノリボンの新しい電気伝導特性を発見

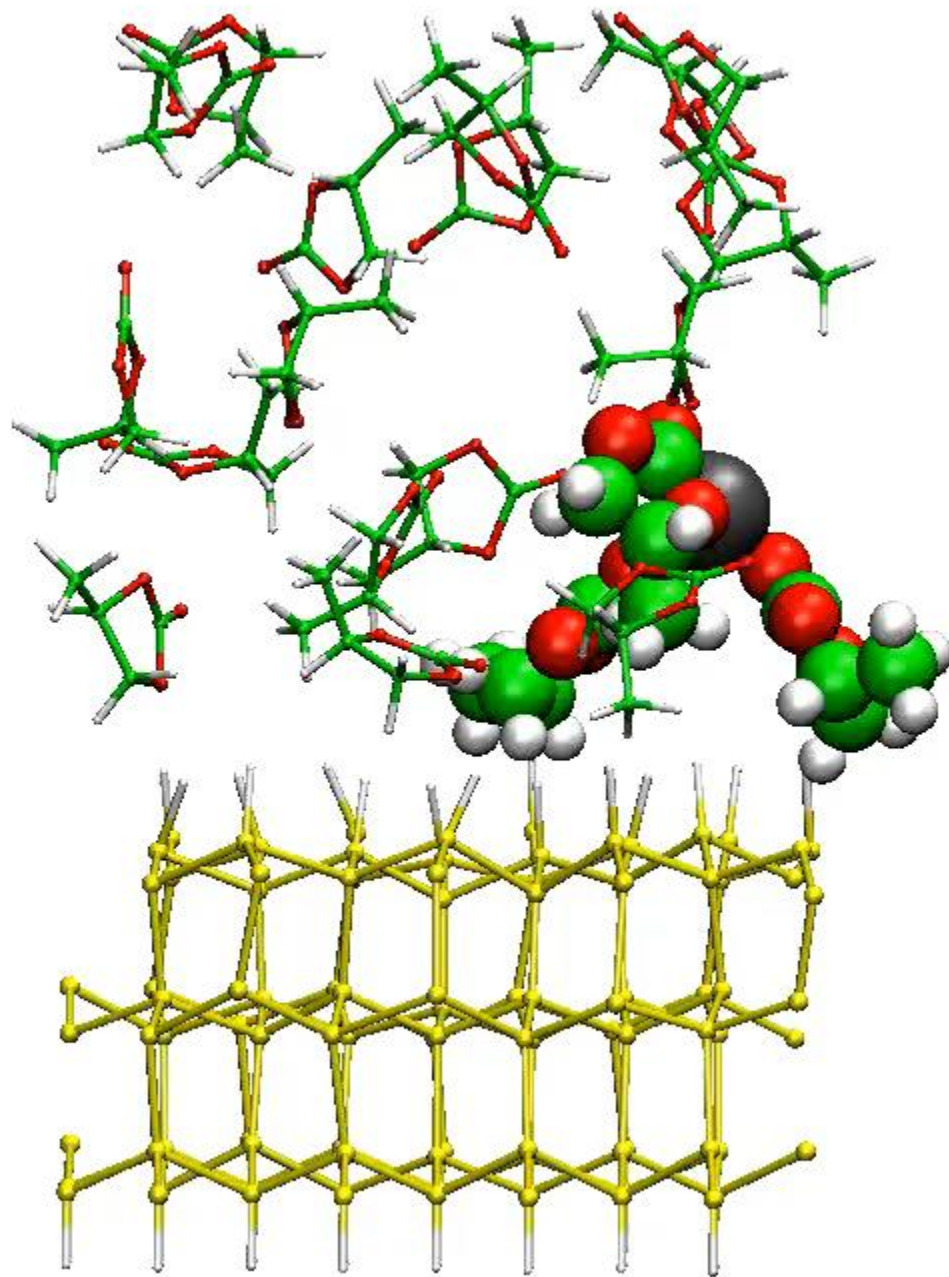




# リチウムイオン 電池の充電過程 を理解する



<http://ev.nissan.co.jp/LEAF/PERFORM>





# シミュレーションによる物質科学 ≡ 現代の錬金術



<http://www.abundancetapestry.com/awaken-your-inner-chemist/>