Inhomogeneous Phase and Phase Transitions Driven by Competing Interactions of Br Atoms Adsorbed on Cu(111) Surface

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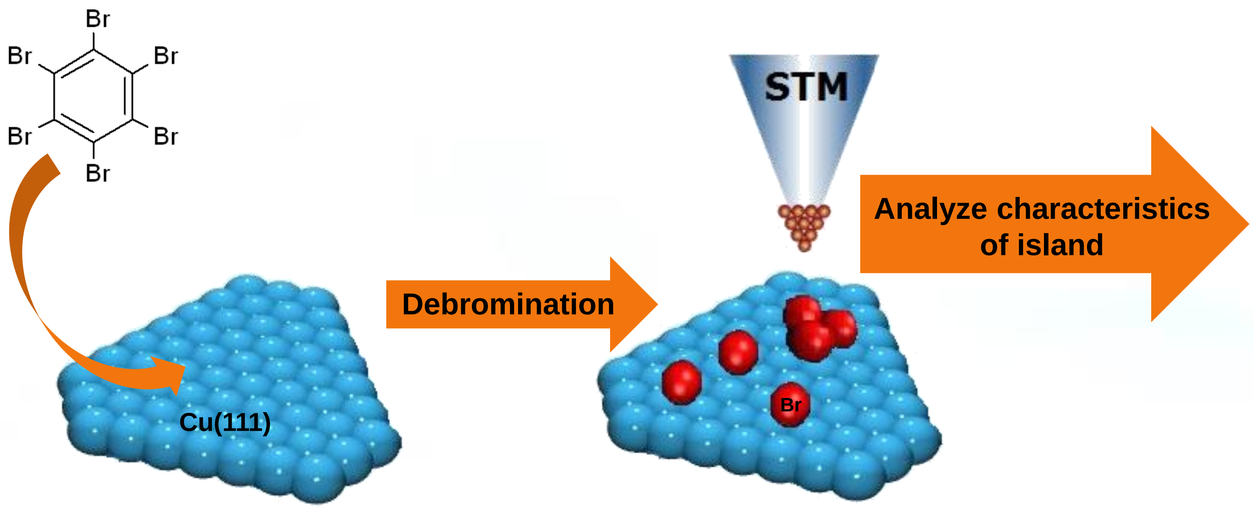
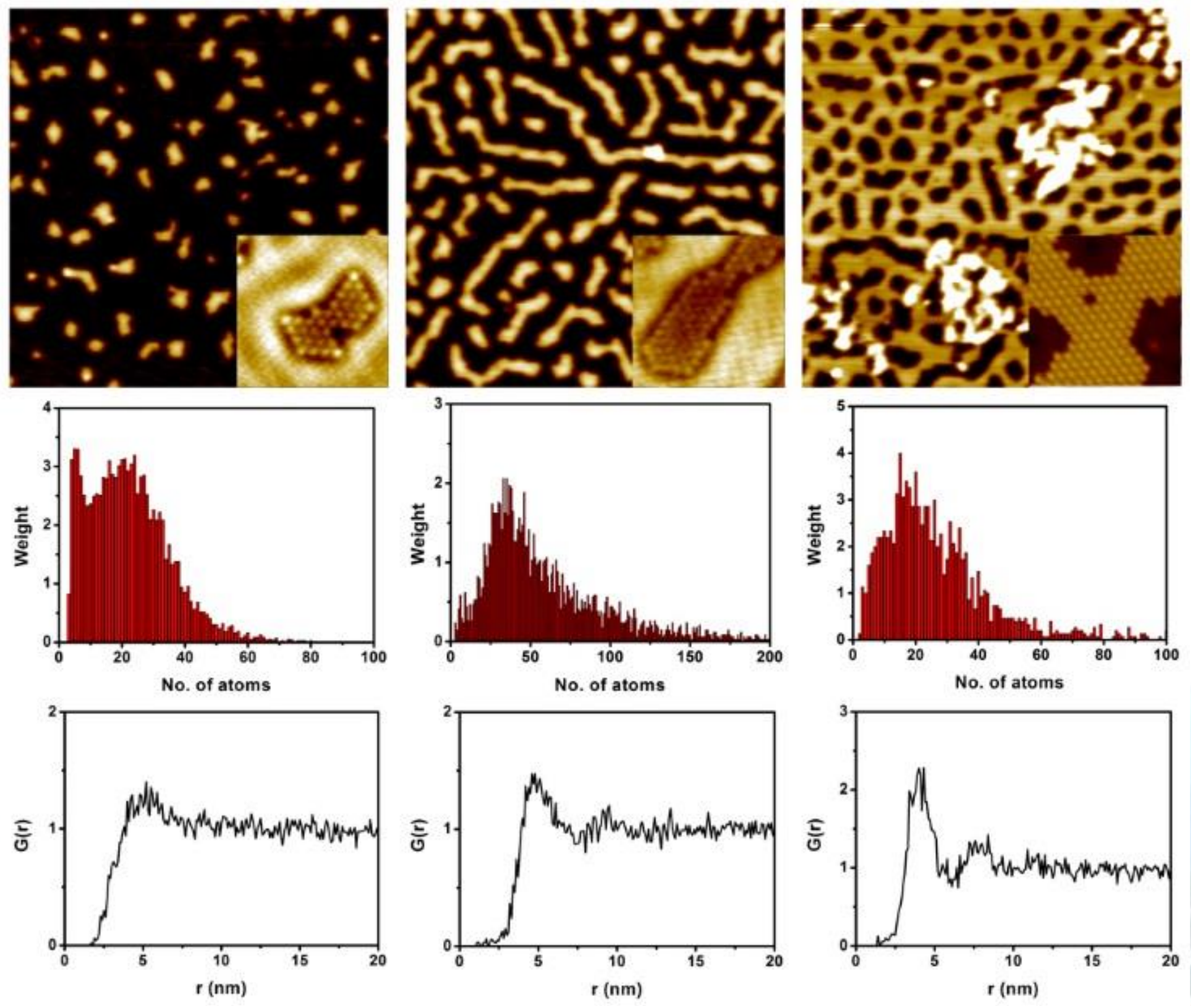
Experiment



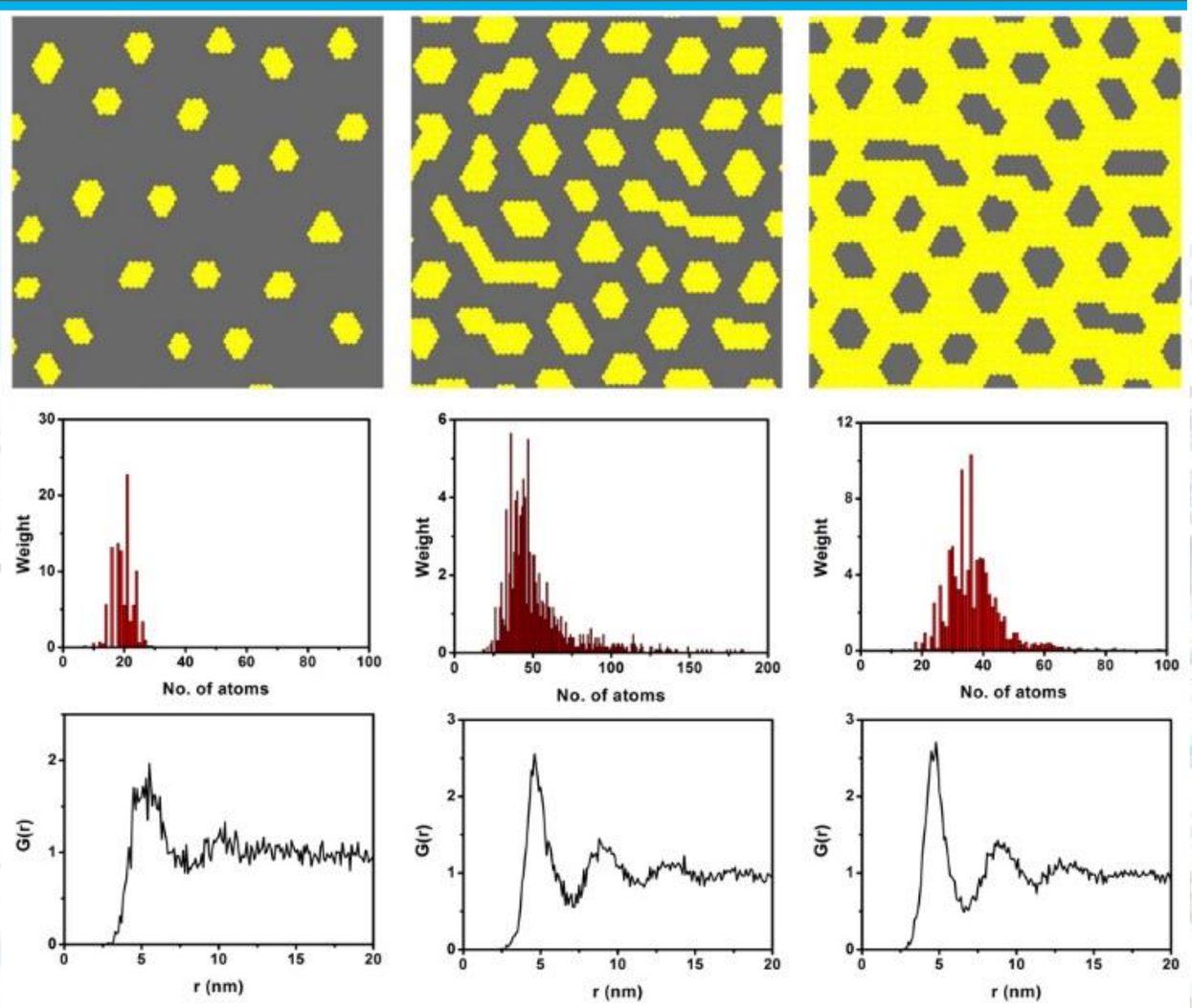
- The experiments were operated at cryogenic temperature (4.9 K) and ultra-high vacuum condition (~10^{-10} mbar). The Br adatoms were introduced by depositing hexabromobenzene onto Cu(111) surface at low temperature. After deposition, hexabromobenzene molecules were dissociated to form phenyl intermediates and Br adatoms.

STM / Island Analysis



- The panels present STM images, size distributions and pair correlation functions of three experimental trials with different coverage of Br atoms, respectively.
- The cases with coverage 10.92%, 33.65% and 71.95%, respectively, are listed from left to right. In calculation of size distribution and pair correlation, the island in first two configurations and the hole in last configuration were taken into account.

Monte Carlo Simulation



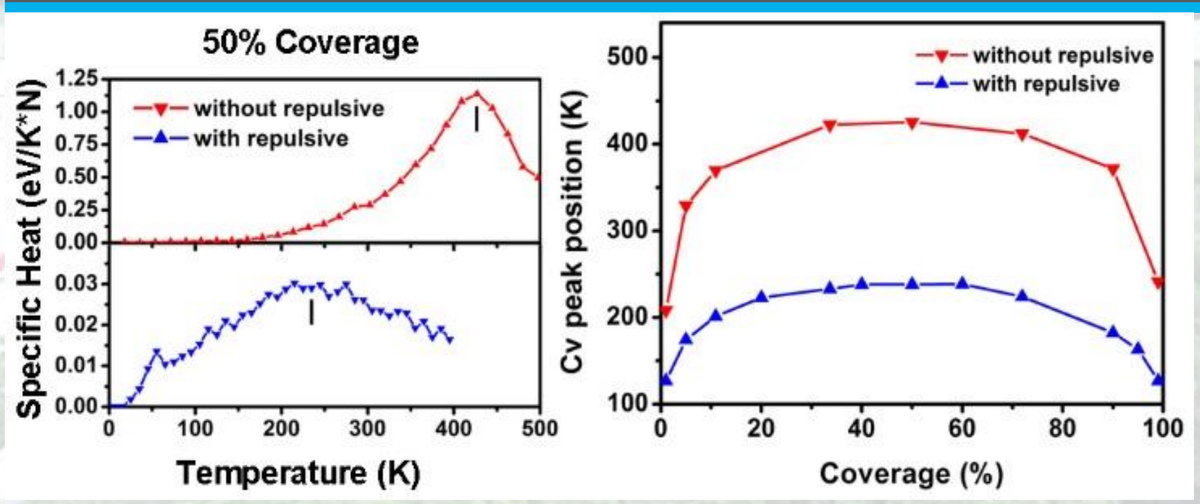
- Monte Carlo simulation is used to reproduce experimentally-observed phase evolution at three different coverage.
- The total energy of the system is formulated as:

$$-U = \frac{1}{2}\left(J_A \sum_{r,r'}^{|r-r'|=1} S_r S_{r'} - J_B \sum_{r,r'} \frac{S_r S_{r'}}{|r-r'|^3} \right)$$

J_A defines the attractive interaction between bromine atoms; J_B defines the long-range dipole-dipole repulsive interaction; S_i=1 (0) when site i is occupied (unoccupied) by a Br atom.

- Based on the DFT results, we set J_A=42 meV. When J_B is set as 7 meV, the simulations can satisfactorily reproduce the main characteristics observed experimentally.

Study of Phase Transition



- To study the phase transition, we carried out MC simulations to simulate the specific heat with different coverages. To make a comparison, the specific heat of system without the long-range repulsion is also simulated.
- We observed that these two systems exhibit very different characteristics: the long-range repulsion lowers the transition temperature and broadens the transition peaks.

Conclusion

- In conclusion, we investigated the inhomogeneous phase and phase transition of bromine atoms on Cu(111) using STM and MC simulation.