## Dr. Lin-Wang Wang, Senior Staff Scientist Lawrence Berkeley National Laboratory



Bio: Lin-Wang Wang: Senior Staff Scientist, Lawrence Berkeley National Laboratory, Berkeley, CA, U.S. Dr. Wang has 25 years of experience in large scale electronic structure calculations. He has worked in O(N) electronic structure calculations in early 1990s. Worked with Alex Zunger, he invented the folded spectrum method which pushed the limit of nonselfconsistent electronic structure calculations from 100 atoms to thousands of atoms. He developed a linear combination of bulk bands (LCBB) method for semiconductor heterostructrure electronic structure calculations, which allows the calculation of million atom devices. He developed generalized moments method which calculates the density of state and optical absorption spectra of a given system without explicit calculation of its eigenstates. He also developed a popular parallel total energy plane wave pseudopotential program (PEtot). He

invented a charge patching method, which enables the ab initio accuracy thousand atom calculations for nanosystems. He has developed a linear scaling three dimensional fragment method (LS3DF), which can be used to selfconsistently calculate systems with tens of thousands of atoms. Recently, he developed a new algorithm for real-time time-dependent DFT calculations which accelerates the traditional algorithms by hundreds of times.

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