**First-principles study of Electric-field induced *Z*2 topological phase transition in strained one-bilayer Bi(111)**

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　Electric-field induced *Z*2 topological phase transition is important for applications of a *Z*2 topological insulator. If we are able to switch from *Z*2 topological insulating phase to trivial insulating phase or vice versa by the electric field, novel devices using edge spin currents could be realized. We predicted that one-bilayer Bi(111) shows electric-field induced *Z*2 topological phase transition by first-principles calculations[1]. The bandgap is closed at the electric field *E* = 2.1 V/Å and one-bilayer Bi(111) shows *Z*2 topological phase transition from *Z*2 topological insulating phase (*E*  < 2.1 V/Å) to trivial insulating phase (*E*  > 2.1 V/Å). In order to realize device applications, the critical electric field should be reduced by tuning the bandgap.
　In this study, we performed fully relativistic density functional calculations of the bandgap and *Z*2 topological invariant in strained one-bilayer Bi(111) shown in Fig. (a). In order to compute *Z*2 topological invariant using OpenMX code [2], we have implemented Fukui-Hatsugai method[3] which can be applied to the system without space inversion symmetry. Figure (b) shows the *Z*2 topological phase diagram of one-bilayer Bi(111) in the space of the electric field and strain with the 3D plot of the band structure at the strain 0.5 %. The bandgap of one-bilayer Bi(111) is closed at the strain 0.5 %, and quadratic band touching[4] appears at Γ point. Near the strain 0.5 %, the critical electric field is reduced to *E* < 1.0 V/Å. In the poster session, we will present our detailed calculated results and how to implement Fukui-Hatsugai method in OpenMX code.

Figure: (a) The structure of one-bilayer Bi(111) (b) The *Z*2 topological phase diagram with the 3D plot of quadratic band touching at the strain 0.5 %

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