Extending Crystallographic Foundations of Materials

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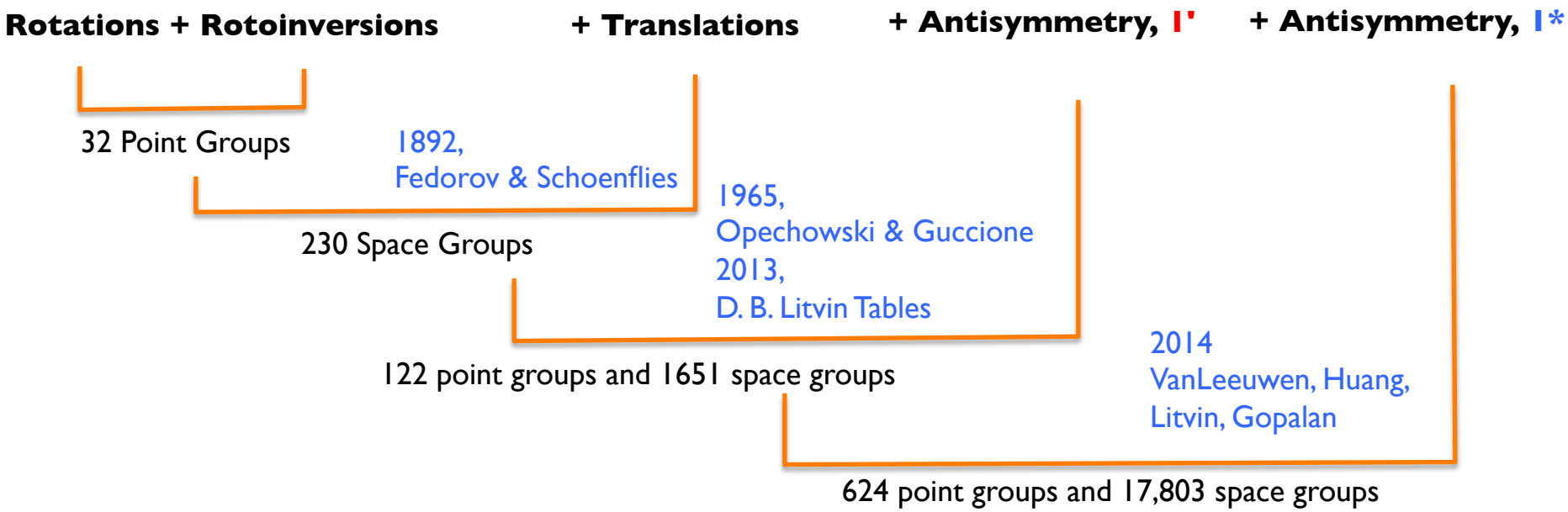

Crystallography is a foundation of our understanding of crystalline materials. The above schematic depicts the evolution of our complete knowledge of the 230 conventional space groups over a century ago, and of 1651 magnetic groups a half century ago by the includiong of time reversal antisymmetry, 1'. By including a second antisymmetry, 1*, the 17803 groups thus generated were recently listed by the Penn State team. The full listing of the double antisymmetry space groups can be found in the supplementary materials of the references below and at http://sites.psu.edu/gopalan/research/symmetry/. Gopalan and Litvin introduced *Rotation-reversal symmetry*, 1*, to generalize the symmetry classification of rigid static rotations in crystals (Gopalan, V. & Litvin, D. B. (2011). Nat. Mater. 10, 1–6). These symmetry groups have the potential to advance understanding of polyhedral rotations in crystals, the magnetic structure of distorted crystals, interfaces, domain walls, and aid in the design of new metamaterials.

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