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Topological Quantum Chemistry III: Topological data mining based on band connectivity MAIA VERGNIORY, Donostia International Physics Center, Donostia-San Sebastian, 20018 Spain, BARRY BRADLYN, JEN-NIFER CANO, Princeton Center for Theoretical Science, Princeton University, Princeton, New Jersey 08544, USA, ZHIJUN WANG, Department of Physics, Princeton University, Princeton, New Jersey 08544, USA, LUIS ELCORO, MOIS AROYO, Department of Condensed Matter Physics, University of the Basque Country UPV/EHU, Apartado 644, 48080 Bilbao, Spain, CLAUDIA FELSER, Max Planck Institute for Chemical Physics of Solids, 01187 Dresden, Germany, BOG-DAN ANDREI BERNEVIG, Department of Physics, Princeton University, Princeton, New Jersey 08544, USA — In this talk I will present the theory and implementation to calculate and tabulate the band connectivity for every orbital of all elements that can appear in materials database of the 230 space groups and that can sit at every Wyckoff position allowed by that group. Using this tables we can predict all the topological semimetals and topological insulators (including time reversal, symmorphic and non symmorphic) that we can find in any database.

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