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Design of half-metallic antiferromagnets: transition metal chalcogenides and pnictides HISAZUMI AKAI, MASAKO OGURA, Department of Physics, Osaka University, NGUYEN HOANG LONG, ISSP, University of Tokyo — Half-metallic antiferromagnts are the materials that exhibit half-metallicity and antifirromagnetism (compensated ferrimagnetism) simultaneously. Such materials are especially useful for spintronics devices since they have 100 % spin-polarized Fermi surfaces despite of their robustness against a disturbance of external magnetic field. We found that (XY)Z_2, where X and Y are transition metal elements and Z is a chalcogens or a pnictigen, show half-metallic antiferromagnetism when the sum of effective d electron numbers of X and Y is 10. Examples are (CrFe)S_2 and (CrFe)Se_2. We report a systematic investigation of the electronic structure and transport properties of these materials calculated by the KKR-Green's function method combined with the Kubo-Greenwood formula.

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