

Simon Steinberg

List of Publications by Year in descending order

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#	ARTICLE	IF	CITATIONS
1	The Crystal Orbital Hamilton Population (COHP) Method as a Tool to Visualize and Analyze Chemical Bonding in Intermetallic Compounds. <i>Crystals</i> , 2018, 8, 225.	2.2	199
2	Development of a robust tool to extract Mulliken and Löwdin charges from plane waves and its application to solid-state materials. <i>RSC Advances</i> , 2019, 9, 29821-29830.	3.6	77
3	Unexpected Ge ⁴⁺ Ge Contacts in the Two-Dimensional Ge ₄ Se ₃ Te Phase and Analysis of Their Chemical Cause with the Density of Energy (DOE) Function. <i>Angewandte Chemie - International Edition</i> , 2017, 56, 10204-10208.	13.8	64
4	Discovering Electron-Transfer-Driven Changes in Chemical Bonding in Lead Chalcogenides (PbX, where X = S, Se, Te). <i>Chemistry of Materials</i> , 2019, 31, 2100-2106.	21.0	56
5	High-Pressure NiAs-Type Modification of FeN. <i>Angewandte Chemie - International Edition</i> , 2017, 56, 7302-7306.	13.8	43
6	Cation-Poor Complex Metallic Alloys in Ba(Eu)AuAl(Ga) Systems: Identifying the Keys that Control Structural Arrangements and Atom Distributions at the Atomic Level. <i>Inorganic Chemistry</i> , 2015, 54, 10296-10308.	4.0	30
7	Identifying a Structural Preference in Reduced Rare-Earth Metal Halides by Combining Experimental and Computational Techniques. <i>Inorganic Chemistry</i> , 2012, 51, 11356-11364.	4.0	29
8	Magnetocaloric Behavior in Ternary Europium Indides Eu ₅ In: Probing the Design Capability of First-Principles-Based Methods on the Multifaceted Magnetic Materials. <i>Chemistry of Materials</i> , 2017, 29, 2599-2614.	6.7	29
9	Revealing Tendencies in the Electronic Structures of Polar Intermetallic Compounds. <i>Crystals</i> , 2018, 8, 80.	2.2	27
10	Long-Range Forces in Rock-Salt-Type Tellurides and How they Mirror the Underlying Chemical Bonding. <i>Advanced Materials</i> , 2021, 33, e2100163.	21.0	26
11	From the Ternary Eu(Au/In) ₂ and EuAu ₄ (Au/In) ₂ with Remarkable Au/In Distributions to a New Structure Type: The Gold-Rich Eu ₅ Au ₁₆ (Au/In) ₆ Structure. <i>Inorganic Chemistry</i> , 2015, 54, 8187-8196.	4.0	23
12	Search for the Mysterious Si ⁴⁺ Te System Using First-Principles-Based Methods. <i>Crystal Growth and Design</i> , 2016, 16, 6152-6155.	3.0	23
13	Electron Counting Rules and Electronic Structure in Tetrameric Transition-Metal (T)-Centered Rare-Earth (R) Cluster Complex Halides (X). <i>Inorganic Chemistry</i> , 2015, 54, 1026-1037.	4.0	22
14	The Proliferous {Zr ₆ X ₁₂ R} and {Zr ₆ X ₁₀ R} Structure Types with Isolated Endohedrally Stabilized (Z) Rare-Earth Metal (R) Cluster Halide (X) Complexes. <i>Zeitschrift Fur Anorganische Und Allgemeine Chemie</i> , 2012, 638, 1922-1931.	1.2	21
15	Crystal Structure and Bonding in BaAu ₅ Ga ₂ and AeAu _{4+x} Ga ₃ (Ae = Ba and Eu): Hexagonal Diamond-Type Au Frameworks and Remarkable Cation/Anion Partitioning in the AeAu ⁺ Au ⁻ Ga Systems. <i>Inorganic Chemistry</i> , 2015, 54, 1010-1018.	4.0	21
16	Revisiting the Si ⁴⁺ Te System: SiTe ₂ Finally Found by Means of Experimental and Quantum-Chemical Techniques. <i>Inorganic Chemistry</i> , 2017, 56, 11398-11405.	4.0	21
17	Gold-rich R ₃ Au ₇ Sn ₃ : establishing the interdependence between electronic features and physical properties. <i>Journal of Materials Chemistry C</i> , 2015, 3, 8311-8321.	5.5	20
18	Breaking the paradigm: record quindecim charged magnetic ionic liquids. <i>Materials Horizons</i> , 2017, 4, 217-221.	12.2	20

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19	Revealing the Nature of Bonding in Rare-Earth Transition-Metal Tellurides by Means of Methods Based on First Principles. <i>European Journal of Inorganic Chemistry</i> , 2017, 2017, 3395-3400.	2.0	19
20	Gold in the Layered Structures of $R_3Au_7Sn_3$: From Relativity to Versatility. <i>Crystal Growth and Design</i> , 2016, 16, 5657-5668.	3.0	18
21	The Mineral St $\frac{1}{4}$ tzite: a Zintl-Phase or Polar Intermetallic? A Case Study Using Experimental and Quantum-Chemical Techniques. <i>Inorganic Chemistry</i> , 2018, 57, 412-421.	4.0	17
22	Fermi-Level Characteristics of Potential Chalcogenide Superconductors. <i>Chemistry of Materials</i> , 2018, 30, 2251-2261.	6.7	15
23	Bonding diversity in rock salt-type tellurides: examining the interdependence between chemical bonding and materials properties. <i>RSC Advances</i> , 2021, 11, 20679-20686.	3.6	14
24	Revealing the Nature of Chemical Bonding in an $Al_nAg_3Te_5$ -Type Alkaline-Metal (A) Lanthanide (Ln) Silver Telluride. <i>Inorganics</i> , 2019, 7, 70.	2.7	12
25	Revisiting the Zintl-Klemm Concept for $Al_nAg_3Te_5$ -Type Alkaline-Metal (A) Lanthanide (Ln) Silver Tellurides. <i>Crystals</i> , 2020, 10, 184.	2.2	12
26	Approaching the Glass Transition Temperature of GeTe by Crystallizing $Ge_{15}Te_{85}$. <i>Physica Status Solidi - Rapid Research Letters</i> , 2021, 15, 2000478.	2.4	12
27	Probing the Validity of the Zintl-Klemm Concept for Alkaline-Metal Copper Tellurides by Means of Quantum-Chemical Techniques. <i>Materials</i> , 2020, 13, 2178.	2.9	11
28	Revealing the Bonding Nature in an Al_nZnTe_3 -Type Alkaline-Metal (A) Lanthanide (Ln) Zinc Telluride by Means of Experimental and Quantum-Chemical Techniques. <i>Crystals</i> , 2020, 10, 916.	2.2	10
29	Eu_2CuSe_3 Revisited by Means of Experimental and Quantum-Chemical Techniques. <i>European Journal of Inorganic Chemistry</i> , 2021, 2021, 1510-1517.	2.0	9
30	Change of magnetic and electronic features through subtle substitution in cubic, non-centrosymmetric extended rare-earth metal cluster complexes $\{TR\}_3X_3$. <i>Journal of Solid State Chemistry</i> , 2013, 206, 176-181.	2.9	7
31	Identifying the Origins of Vacancies in the Crystal Structures of Rock Salt-type Chalcogenide Superconductors. <i>ACS Omega</i> , 2019, 4, 15721-15728.	3.5	7
32	Examination of a Structural Preference in Quaternary Alkali-Metal (A) Rare-Earth (R) Copper Tellurides by Combining Experimental and Quantum-chemical Means. <i>Inorganic Chemistry</i> , 2022, 61, 9269-9282.	4.0	6
33	Oligomeric rare-earth metal cluster complexes with endohedral transition metal atoms. <i>Journal of Solid State Chemistry</i> , 2014, 219, 159-167.	2.9	5
34	Layered Structures and Disordered Polyanionic Nets in the Cation-Poor Polar Intermetallics $CsAu_{1.4}Ga_{2.8}$ and $CsAu_2Ga_{2.6}$. <i>Crystal Growth and Design</i> , 2017, 17, 693-700.	3.0	4
35	Exploring the frontier between polar intermetallics and Zintl phases for the examples of the prolific Al_nTnTe_3 -type alkali metal (A) lanthanide (Ln) late transition metal (Tn) tellurides. <i>Zeitschrift Fur Naturforschung - Section B Journal of Chemical Sciences</i> , 2021, 76, 635-642.	0.7	4
36	$Rb_3Er_4Cu_5Te_{10}$: exploring the frontier between polar intermetallics and Zintl phases via experimental and quantumchemical approaches. <i>European Journal of Inorganic Chemistry</i> , 0, .	2.0	4

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37	Eine NiAs-artige Hochdruckmodifikation von FeN. <i>Angewandte Chemie</i> , 2017, 129, 7408-7412.	2.0	2
38	Nickel hexayttrium decaiodide, [NiY ₆]I ₁₀ . <i>Acta Crystallographica Section E: Structure Reports Online</i> , 2014, 70, i26-i26.	0.2	1
39	Lead Chalcogenides: Discovering Electron-Transfer-Driven Changes in Chemical Bonding in Lead Chalcogenides (PbX, where X = Te, Se, S, O) (<i>Adv. Mater.</i> 49/2020). <i>Advanced Materials</i> , 2020, 32, 2070370.	21.0	1
40	Sr ₇ N ₂ Sn ₃ : a layered antiperovskite-type nitride stannide containing zigzag chains of Sn ₄ polyanions. <i>Zeitschrift Fur Naturforschung - Section B Journal of Chemical Sciences</i> , 2021, .	0.7	1
41	Chemical Reactions and Phase Stabilities in the Si-Te System at High Pressures and High Temperatures. <i>Inorganic Chemistry</i> , 2022, 61, 7349-7357.	4.0	0