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Editorial

Special Issue on "Recent Advances in Novel Materials for Future Spintronics"

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1. Referees for the Special Issue

A total of 23 manuscripts were received for our Special Issue (SI), of which 7 manuscripts were directly rejected without peer review. The remaining 16 articles were all strictly reviewed by no less than two reviewers in related fields. Finally, 13 of the manuscripts were recommended for acceptance and published in *Applied Sciences-Basel*. Referees from 10 different countries provided valuable suggestions for the manuscripts in our SI, the top five being the USA, Germany, Korea, Spain, and Finland. The names of these distinguished reviewers are listed in Table A1. We would like to thank all of these reviewers for their time and effort in reviewing the papers in our SI.

2. Main Content of the Special Issue

Since tetragonal Heusler compounds have many potential applications in spintronics and magnetoelectric devices, such as ultrahigh-density spintronic devices, spin transfer torque devices, and permanent magnets, they have received extensive attention in recent years [1–5]. In this SI, Zhang et al. [6] studied the magnetic and electronic structures of cubic and tetragonal types of Mn_3Z (Z = Al, Ga, In, Tl, Ge, Sn, Pb) Heusler alloys. The authors used first-principles calculations to describe the impact of increasing atomic radius on the structure and properties of Heusler alloys. They investigated tetragonal distortions in relation to different volumes for Mn_3Ga alloys and extended this analysis to other elements by replacing Ga with Al, In, Tl, Si, Ge, Sn, and Pb.

Spintronics has many advantages over traditional electronics, such as no volatility, high data processing speed, low energy consumption, and high integration density. Therefore, spintronics, which utilizes spin instead of charge as the carrier for information transportation and processing, can be seen as one of the most promising ways to implement high-speed and low-energy electronic devices. However, in the process of developing spintronic devices, we have also encountered many bottlenecks, including spin-polarized carrier generation and injection, long-range spin-polarization transport, and spin manipulation and detection. To overcome these problems, various types of spintronic materials have been proposed, such as spin-gapless semiconductors (SGSs) [7–13], Dirac half-metals [14,15], diluted magnetic semiconductors (DMSs) [16,17], and bipolar magnetic semiconductors (BMSs) [18–20]. In this SI, Liu et al. [21] predicted two new 1:1:1:1 quaternary Heusler alloys, ZrRhTiAl and ZrRhTiGa, and studied their mechanical, magnetic, electronic, and half-metallic properties via first principles. Chen et al. [22] investigated the effect of main-group element doping on the magnetism, half-metallic property, Slater–Pauling rule, and electronic structures of the TiZrCoIn alloy. Feng et al. [23] calculated the band structures, density of states, magnetic moments, and the band-gap of two quaternary Heusler half-metals, FeRhCrSi and FePdCrSi, by means of first principles. Zhang et al. [24] performed first-principles calculation to investigate the electronic structure of half-metallic Prussian blue analogue

$GaFe(CN)_6$. They revealed its magnetic and mechanical properties. The pressure dependence of the electronic structure was also investigated in their study. In 2017, Wang et al. [25] predicted a rare strain-tunable electronic band structure, which can be utilized in spintronics. Based on Wang et al.'s study, Chen et al. [26] demonstrated that the physical state of ScFeRhP can be tuned by uniform strain. Theoretical predictions of strain-adjustable quaternary spintronic Heusler compounds remain of high importance in the field of spintronics. Similar works can also be found in References [27–32].

In recent years, SGSs [33] have attracted widespread attention in the field of spintronics. Thus far, nearly 100 Heusler-type SGSs have been theoretically predicted, of which Mn_2CoAl, Ti_2CoAl, and Ti_2CoSi have been extensively studied. In this SI, Wei, Wu, and Feng et al. focused on these novel materials. Wei et al. [34] studied the interfacial electronic, magnetic, and spin transport properties of $Mn_2CoAl/Ag/Mn_2CoAl$ current-perpendicular-to-plane spin valves (CPP-SV) based on density functional theory and non-equilibrium Green's function. Wu et al. [35] conducted a comprehensive study of the electronic and magnetic properties of the Ti_2CoAl/MgO (100) heterojunction with first-principles calculations. Ten potential Ti_2CoAl/MgO (100) junctions are presented based on the contact between the possible atomic interfaces. The atom-resolved magnetic moments at the interface and subinterface layers were calculated and compared with the values obtained from bulk materials. The spin polarizations were calculated to further illustrate the effective range of tunnel magnetoresistance (TMR) values. Feng et al. [36] systematically investigated the effect of Fe doping in Ti_2CoSi and observed the transition from gapless semiconductor to nonmagnetic semiconductor.

Chen et al. [37] used the spin-polarized density functional theory based on first-principles methods to investigate the electronic and magnetic properties of bulk and monolayer $CrSi_2$. Their calculations show that the bulk form of $CrSi_2$ is a nonmagnetic semiconductor with a band gap of 0.376 eV. Interestingly, there are claims that the monolayer of $CrSi_2$ is metallic and ferromagnetic in nature, which is attributed to the quantum size and surface effects of the monolayer.

Jekal et al. [38] conducted a theoretical investigation with the help of the density functional theory and showed that the creation of small, isolated, and stabilized skyrmions with an extremely reduced size of a few nanometers in $GdFe_2$ films can be predicted by 4d and 5d TM (transition metal) capping. Magnetic skyrmions is an exciting area of research and has gained much attention from researchers all over the world. We hope that this work may add value to the scientific community and be helpful for reference in future work.

Finally, we introduce two manuscripts in this SI related to computational materials. Although these two papers are not in the field of spintronics, they belong to the field of computational materials science. The interaction of hydrogen with metal surfaces is an interesting topic in the scientific and engineering world. In this SI, Wu et al. [39] investigated the hydrogen adsorption and diffusion processes on a Mo-doped Nb (100) surface and found that the H atom is stabilized at the hollow sites. They also evaluated the energy barrier along the HS→TIS pathway. Due to their unique physical properties and wide application, Bi-based oxides have received extensive attention in the fields of multiferroics, superconductivity, and photocatalysis. In this SI, Liu et al. [40] investigated the electronic structure as well as the optical, mechanical, and lattice dynamic properties of tetragonal $MgBi_2O_6$ using the first-principles method.

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Conflicts of Interest: The authors declare no conflict of interest.

Appendix A

Table A1. SI reviewer list.

Antonio Frontera	Attila Kákay	Anton O. Oliynyk	Akinola Oyedele
Bhagwati Prasad	David L. Huber	Élio Alberto Périgo	Guangming Cheng
Hannes Rijckaert	Jae Hoon Jang	Jesús López-Sánchez	Ji-Sang Park
Kaupo Kukli	Lalita Saharan	Marijan Beg	Michael Leitner
Masayuki Ochi	Ning Kang	Norbert M. Nemes	Supriyo Bandyopadhyay
Shuo Chen	Soumyajyoti Haldar	Suranjan Shil	Torbjörn Björkman
Uwe Stuhr	Weon Ho Shin	Xueqiang Alex Zhang	Masayuki Ochi
Byeongchan Lee			

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