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Jun-Wei Luo, Shu-Shen Li, and Alex Zunger

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# Rapid transition of the hole Rashba effect from strong field dependence to saturation in semiconductor nanowires

Jun-Wei Luo,<sup>1,2,3,\*</sup> Shu-Shen Li,<sup>1,2,3</sup> and Alex Zunger<sup>4,†</sup>

<sup>1</sup>*State key laboratory of superlattices and microstructures,  
Institute of Semiconductors, Chinese Academy of Sciences, Beijing 100083, China*

<sup>2</sup>*College of Materials Science and Opto-Electronic Technology,  
University of Chinese Academy of Sciences, Beijing 100049, China*

<sup>3</sup>*Synergetic Innovation Center of Quantum Information and Quantum Physics,  
University of Science and Technology of China, Hefei, Anhui 230026, China*

<sup>4</sup>*Renewable and Sustainable Energy Institute,  
University of Colorado, Boulder, Colorado 80309, USA*

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## Abstract

The electric field manipulation of the Rashba spin-orbit coupling effects provides a route to electrically control spins, constituting the foundation of the field of semiconductor spintronics. In general, the strength of the Rashba effects depends linearly on the applied electric field and is significant only for heavy-atom materials with large intrinsic spin-orbit interaction under high electric fields. Here, we illustrate in 1D semiconductor nanowires an anomalous field-dependence of the hole (but not electron) Rashba effect (HRE): (i) At low fields the strength of the HRE exhibits a steep increase with field so even low fields can be used for device switching. (ii) At higher fields the HRE undergoes a rapid transition to saturation with a giant strength even for light-atom materials such as Si (exceeding 100 meVÅ). (iii) The nanowire size-dependence of the saturation HRE is rather weak for light-atom Si so size fluctuations would have a limited effect, a key requirement for scalability of Rashba field-based spintronic devices. This offers Si nanowires as a promising platform for the realization of scalable CMOS-compatible spintronic devices.

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\* jwluo@semi.ac.cn

† Alex.Zunger@colorado.edu

Coherent manipulations of electron spins in semiconductors by electrical means have been demonstrated [1–5], however, it has proven difficult to find in tetrahedral semiconductors a strong Rashba effect, which is apparently needed for achieving efficient spin manipulation [5–7] in the Rashba effect-based spintronics devices [1, 2, 8]. This difficulty has stimulated searches of strong Rashba effect in non-standard non-tetrahedral 3D materials [9–11] that tend, however, to be incompatible with current semiconductor technology. Thus far, studies of electrical manipulation of spins using the Rashba effect have focused mostly on the electron Rashba effect (ERE), which is a third-order effect, leading to rather modest ERE as illustrated in Figure 1 for InAs 1D nanowires as a function of either applied electric field (Fig. 1a) or nanostructure dimension (Fig. 1b). Not only is the Rashba effect weak for electrons, but electrons strongly coupling to nuclear spins, producing high decoherence rates, whose control remains the biggest challenge in quantum information hardware [2, 6, 12].

On the other hand, hole spins in semiconductors have weak coupling to nuclear spins, and therefore, have the potential for longer coherence times [2, 12]. The reason that nevertheless there are but very few studies of hole Rashba effect (HRE) in semiconductors [2, 7, 12–15] is likely because of the earlier focus on 2D systems, in which holes exhibit short spin lifetime [6] and negligible Rashba effect owing to the lack of the  $k$ -linear spin splitting [13, 14]. These two limiting factors have recently been overcome by replacing 2D semiconductor systems with 1D semiconductor nanowires [1–3, 16]. In Ge/Si core/shell nanowires, experimentalists have observed extremely long hole spin relaxation time  $T_1 = 0.6$  ms [2] and hole spin dephasing time  $T_2 = 0.18$   $\mu$ s [7]. A ‘giant’ HRE in 1D nanowires has also recently been noted theoretically in band structure calculations [17] (footnote [25] therein), and discussed by a qualitative model Hamiltonian theory [18], pointing to the possibility of a direct, first-order dipolar coupling of the 1D hole states to the applied electric field. Such dipolar coupling yields a direct Rashba effect with a Hamiltonian  $H_{\text{DR}} = eE_x U \tau_x \sigma_z$  (where  $E_x$  is applied electric field perpendicular to nanowires,  $U = \langle \psi_{h0\pm} | (-x) | \psi_{h1\pm} \rangle$  the dipolar coupling constant between the ground hole  $\psi_{h0\pm}$  and first excited hole  $\psi_{h1\pm}$  states, and  $\tau_i$  and  $\sigma_i$  the Pauli matrices acting on orbital part  $\{\psi_{h0}, \psi_{h1}\}$  and spin part  $\{+, -\}$  of eigenstates, respectively).

The possibility of manipulation of carrier spins via Rashba effect led to many ideas for all electrically controlled spintronic devices such as the Datta-Das spin field-effect transistor (SFET) [8]. However, like the drain current saturation of the field-effect transistor being

essential to reach the maximum possible operating speeds, in practical applications of SFET type devices, saturation of the drain spin current with applied electric field, thus saturation of the Rashba effect is essential, an elusive goal yet to be discovered. In this work, we find that (i) at low electric fields the strength of the Rashba effect for holes depends strongly on the electric field. The field tunable HRE ranging from zero to the large value with an unexpected small electric field is highly desirable for spintronic devices such as Datta-Das SFET. (ii) At intermediate fields the HRE undergoes a rapid transition to saturation with a giant strength even for light-atom materials such as Si. The emergence of the saturation in the HRE ensures the Rashba effect in the saturation regime is immune from inevitable field fluctuations occurring in massive production or scalable applications [19]. These findings will probably boost efforts to further develop SFET [4, 8, 20], spin-orbit qubits [1, 2, 7], and quantum computing using Majorana states [21–25].

**Method: direct evaluation of the strength of the Rashba effect.** We use our previously developed atomistic, material-dependent pseudopotential method to calculate the band structure of semiconductor nanowires under an applied electric field  $\mathbf{E}$  (see supplementary material for details). In the atomistic approach, one does not have to commit at the outset to a linear or non-linear Rashba term, obtaining this information instead, as *output* not *input* from the quantum mechanical description of spin-orbit coupling-induced inter-band coupling. We do not perform self-consistent Schrödinger-Poisson calculations because, as illustrated by Winkler [13] in 2D quantum wells, the strength of the Rashba effect is proportional to the averaged electric field rather than to the local field. Here, the former is an input variable. After solving the Schrödinger equation and obtaining the energy dispersion along  $k_z$  (nanowire along  $z$ ) for nanowires, as shown in Fig. 2a, the spin splitting  $\Delta E_{ss}(i, k_z)$  of the band  $i$  is fit to a power series in  $k_z$ :  $\Delta E_{ss}(i, k_z) = 2\alpha_R^i k_z + \gamma^i k_z^3$ . The coefficients extracted from the fit determine the Rashba parameters  $\alpha_R$  of different subbands [26].

### Electron Rashba effect in 1D nanowires

**(i) Field dependence:** Figure 1 (a) shows the predicted Rashba parameters  $\alpha_R$  of both ERE and HRE in a 15-nm-radius InAs nanowire as a function of applied electric field. We see that the ERE  $\alpha_R$  increases approximately linearly with the electric field and then becomes sublinear when  $E_x > 50$  kV/cm. The deduced ERE coefficient, defined as the slope of  $\alpha_R$  in the linear region, is  $r_{41}^e = \partial\alpha_R/\partial E_x = 90.9$  eÅ<sup>2</sup>, approaching the InAs bulk value of  $r_{41}^{6c6c} = 117.1$  eÅ<sup>2</sup> [13]. At very high fields, ERE  $\alpha_R$  exceeds 100 meVÅ, comparable with

experimentally observed ERE  $\alpha_R = 50 - 100 \text{ meV\AA}$  in 2D InAs QWs or heterostructures [28].

**(ii) Radius dependence:** Fig. 1 (b) shows the radius dependence of the ERE  $\alpha_R$  for InAs nanowires under a fixed electric field of  $E_x = 30 \text{ kV/cm}$ . We see that the ERE  $\alpha_R$  increases initially with nanowire radius  $R$  and then begins to approach the bulk asymptotic value at  $R > 10 \text{ nm}$ . This monotonic, but nonlinear, radius-dependence of the ERE  $\alpha_R$  is similar to the thickness-dependence of the well established ERE in 2D quantum wells, as demonstrated by the best fit (solid line in Fig. 1(b)) to the classical formulation of  $\alpha_R$  developed for 2D electron gases (2DEG) [13]. The ERE  $\alpha_R$  approaches an asymptotic limit

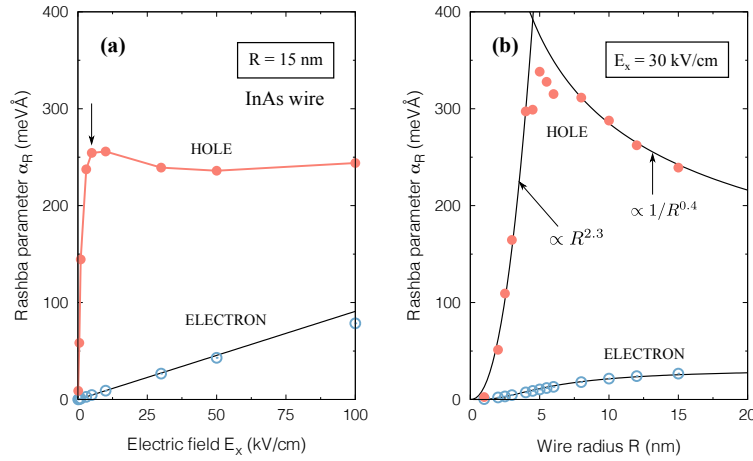


Figure 1. **The strength of the electron and hole Rashba effects in 1D InAs nanowires.**

(a) Predicted Rashba parameter  $\alpha_R$  as a function of electric field for both electrons (open circles) and holes (dots) in a  $R = 15 \text{ nm}$  InAs nanowire, by performing atomistic pseudopotential method calculations. The vertical arrow separates the low field region where HRE depends strongly on field, an effect that can be used beneficially for applications in spintronic devices, and the intermediate field region where field saturation exists. The magnitude of the HRE at saturation is far larger than the ERE, and can reach giant value in nanowires even for light-atom materials such as Si. The black solid line represents a linear fit to electron  $\alpha_R$ . (b) Same as in (a) but as a function of nanowire radius  $R$ , upon application of an electric field  $E_x = 30 \text{ kV/cm}$ . In the case of holes, two solid curves represent the best fit of the rise and fall parts to  $12.9 \times R^{2.3}$  and  $715.9 \times R^{-0.4}$ , respectively. In the case of electrons, the black solid line is the best fit to the well-known bandgap-dependence of the ERE Rashba parameter [27].

of 34 meVÅ as the radius increased, in excellent agreement with expected bulk InAs value of 35 meVÅ under a same field [13]. These agreements with experimental data demonstrate the reliability and validity of the used atomistic method to predict the Rashba effect.

**Giant hole Rashba effect in 1D nanowires with a rapid saturation.** In sharp contrast to the ERE, the red lines in Figure 1 exhibit an unusual size- and field-dependent HRE.

**(i) Field dependence:** In a 15-nm-radius InAs nanowire, Fig. 1(a) shows that as increasing the electric field, the HRE  $\alpha_R$  occurs a steep increase at the weak field, and then quickly saturates (with a saturation  $\alpha_R^{\text{sat}} = 254 \text{ meVÅ}$ ) at a modest field of  $E_x^{\text{sat}} = 5 \text{ kV/cm}$ , as opposed to a mild linear increase of the ERE  $\alpha_R$ . The transition from the steep rise to the saturation occurs within an ultra-small region of the electric field. This rapid saturation of the HRE satisfies the basic requirements for developing practical spintronic devices. The steep rise in the sub-saturation region is linear with a huge slope of about 28000 eÅ<sup>2</sup> (or

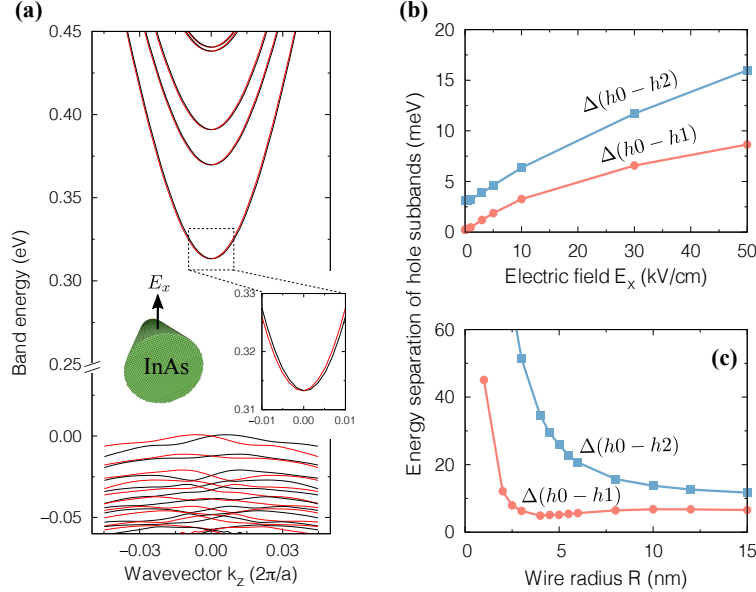


Figure 2. **Energy separations of hole subbands in InAs nanowires.** (a) Band structure of a  $R=15 \text{ nm}$  InAs nanowire under an electric field of 100 kV/cm. Inset is schematic of an InAs nanowire under an electric field. (b) Energy separations of the first excited ( $h1$ ) and second excited ( $h2$ ) hole subbands relative to the ground hole subband ( $h0$ ) at the zone center as a function of electric field  $E_x$  for the  $R = 15 \text{ nm}$  InAs nanowire. (c) Energy separations as a function of nanowire radius  $R$  under an electric field  $E_x = 30 \text{ kV/cm}$ .

termed as the Rashba coefficient  $r_{ss}$ ), which is around 300 times larger than the ERE counterpart. The  $r_{ss}$  is so huge that the HRE  $\alpha_R$  is highly tunable (from zero to  $254 \text{ meV}\text{\AA}$ ) even though it saturates at a modest field. The HRE  $\alpha_R^{\text{sat}}$  reaches a factor of 5 larger than the ERE  $\alpha_R$  at  $E_{\text{sat}} = 5 \text{ kV/cm}$  for the 15-nm-radius InAs nanowire and then reduces toward the higher fields as a result of the saturation of the HRE. The HRE  $\alpha_R^{\text{sat}}$  is 2-5 times larger than reported values of the ERE  $\alpha_R$  in InAs and InSb 2D electron gases [5, 28], and is only one order of magnitude smaller than observed giant Rashba parameters in the polar BiTeI [9] and on the surface of topological insulators [5].

**(ii) Radius dependence:** In compared with the ERE  $\alpha_R$ , the radius-dependence of the HRE  $\alpha_R$  in 1D nanowires is also abnormal and non-monotonic, as shown in Fig. 1 (b). We

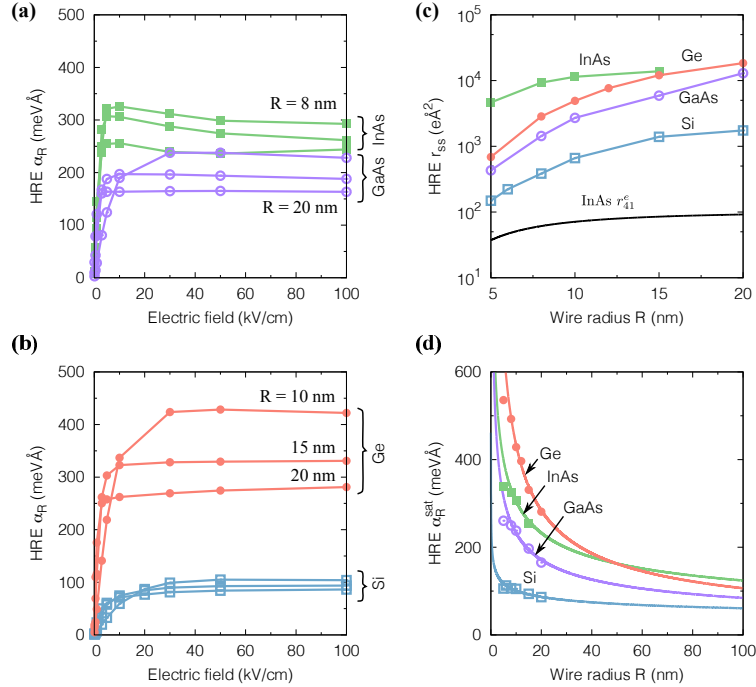


Figure 3. **Electrical response of HRE in nanowires.** HRE  $\alpha_R$  as a function of applied electric field for (a) GaAs and InAs nanowires and (b) Ge and Si nanowires with varying radius  $R$ . (c) Corresponding HRE coefficient  $r_{ss}^h$  in sub-saturation region as a function of nanowire radius  $R$  for InAs, GaAs, Ge, and Si nanowires. The black solid line represents the ERE coefficient  $r_{41}^e$  of InAs nanowires for comparison. (d) Saturation HRE  $\alpha_R^{\text{sat}}$  decays as a  $R^{-\lambda}$  power law toward its asymptotic zero value in bulk. The best fit indicates  $\lambda = 0.39, 0.44, 0.61$ , and  $0.22$  for InAs, GaAs, Ge, and Si nanowire materials, respectively.

see that HRE  $\alpha_R$  increases rapidly as a  $R^{2.3}$  power law, rising faster than the expected linear increase in Ref. [18], and then begins to decrease as a  $R^{-0.4}$  power law once achieving the maximum (a large  $\alpha_R$  of  $\sim 350$  meVÅ). HRE  $\alpha_R$  finally falls to its asymptotic zero value of the heavy-hole band in bulk. Such non-monotonic size-dependent  $\alpha_R$ , to the best of our knowledge, has not been reported in the literature.

**(iii) Material dependence:** The strength of the conventional Rashba effect depends explicitly on two fundamental quantities:  $\Gamma$ -point direct bandgap  $E_g$  and spin-orbit energy  $\Delta_{so}$ , and hence we expect that it is strongest in InAs, modest in GaAs and Ge, but very weak in Si [13]. However, this is not necessary true for the HRE in nanowires since  $\alpha_R$  implicitly depends on  $E_g$  and  $\Delta_{so}$  in the direct Rashba Hamiltonian  $H_{DR}$ . In Figs. 3(a) and (b), we compare predicted HRE  $\alpha_R$  as a function of applied electric field in InAs, GaAs, Ge, and Si nanowires. All nanowires exhibit similar trends of the field-dependent HRE  $\alpha_R$  as in InAs nanowires. Most of the significant features of the hole Rashba effect considered here are within weak electric fields (less than 50 kV/cm), where carrier density is low and hence a self-consistent Poisson-Schrodinger solution is not needed. Indeed, the electric field values required to archive saturation do not extend much beyond the transition point from strong to weak field-dependence (vertical arrow in Fig.1). We summarize deduced HRE  $r_{ss}$  and  $\alpha_R^{\text{sat}}$  in Figs. 3(c) and (d), respectively. We find that both  $r_{ss}$  and  $\alpha_R^{\text{sat}}$  highly, but non-monotonically, depend on  $\Delta_{so}$  and  $E_g$ . Fig. 3(c) shows that the HRE  $r_{ss}$  even in Si nanowires is one order of magnitude larger than ERE  $r_{41}^e$  in InAs nanowires, giving the saturation HRE  $\alpha_R^{\text{sat}}$  in Si nanowires around 110 meVÅ, which is among the largest reported values in InAs and InSb electron systems [5, 28]. HRE  $\alpha_R^{\text{sat}}$  in the saturation regime decays as a  $R^{-\lambda}$  power law toward its asymptotic zero value in bulk. As shown in Fig. 3(d), the decay of the HRE  $\alpha_R^{\text{sat}}$  is rather rapid for GaAs ( $\lambda = 0.44$ ), InAs ( $\lambda = 0.39$ ), and Ge ( $\lambda = 0.61$ ) nanowires, but for light-atom Si nanowires the size dependence is weaker ( $\lambda = 0.2$ ). Thus, for Si nanowires the saturation value of the HRE can be insensitive to size fluctuations over a significant range of sizes, a key requirement for scalability of Rashba field-based spintronic devices.

**The origin of the anomalous HRE in nanowires.** At first glance, we could not understand the anomalous field- and radius-dependences of the HRE  $\alpha_R$  from the direct Rashba Hamiltonian  $H_{DR} = eE_x U \tau_x \sigma_z$  alone since it is apparently linearly proportional to the external field  $E_x$  [18]. We note that  $H_{DR}$  couples with the last term of the effective Luttinger-Kohn Hamiltonian  $H_{LK}^{\text{eff}} = A_+ + A_- \tau_z + C k_z \tau_y \sigma_x$  to lift the otherwise degenerate



hole subbands with  $k$ -linear spin splitting [18], which is a key feature making 1D holes different from electron counterpart as well as 3D bulk and 2D systems. Where  $A_{\pm} = \hbar^2 k_z^2 (m_{h0}^{-1} \pm m_{h1}^{-1}) / 4 \pm \Delta / 2$ , and  $\Delta \propto R^{-2}$  the energy separation between  $h0$  and  $h1$  subbands in the absence of external electric field, arising from the quantum confinement effect. The off-diagonal Hamiltonian matrix  $\langle \psi_{h1\pm} | H_{LK}^{\text{eff}} | \psi_{h0\mp} \rangle = ik_z C$  and hence  $C \propto 1/R$ . We have to diagonalize the Hamiltonian of  $H_{LK}^{\text{eff}} + H_{\text{DR}}$  (neglecting the weak  $H_R$ ) to obtain the spin splitting  $\Delta \epsilon_{ss}(k_z) = 2\alpha_R k_z$  with a Rashba parameter,

$$\alpha_R = \frac{2eCU E_x}{\sqrt{\Delta^2 + 4e^2 U^2 E_x^2}}. \quad (1)$$

The denominator of Eq. (1) is the energy separation between  $h0$  and  $h1$  subbands (or  $h0-h1$  splitting): the first term ( $\Delta$ ) is due to the quantum confinement effect in the absence of the electric field, and the second term arises from the electric field-induced quantum confined Stark effect (QCSE). The competition between these two energy contributions leads to the observed transition between two different electrical responses of the HRE  $\alpha_R$ . If quantum confinement effect dominates the energy separation (i.e.,  $\Delta \gg 2eU E_x$ ),  $\alpha_R \simeq 2eCU E_x / \Delta$ , which is linearly proportional to the electric field  $E_x$ , and if QCSE is predominant (i.e.,  $\Delta \ll 2eU E_x$ ),  $\alpha_R \simeq C$ , which is insensitive to the electric field  $E_x$ . We, therefore, attribute the observed emergence of the saturation of the HRE  $\alpha_R$  to electric field-induced strong QCSE.

We now turn to examine the energy contributions to the  $h0-h1$  splitting. Fig. 2(b) shows the predicted  $h0-h1$  splitting  $\Delta(h0-h1)$  as a function of the electric field for the  $R = 15$  nm InAs nanowire using the atomistic pseudopotential method. For a particular nanowire, the contribution of the quantum confinement effect to the  $h0-h1$  splitting is a constant of  $\Delta$ , which is 0.5 meV for the  $R = 15$  nm InAs nanowire, independent on the applied electric field. We attribute the change of  $\Delta(h0-h1)$  from  $\Delta$  upon application of an electric field to the QCSE. In Fig. 2(b) we see that  $\Delta(h0-h1)$  raises quickly (from 0.5 meV at  $E_x = 0$  to 1.9 meV at  $E_x^{\text{sat}} = 5$  kV/cm) as increasing the electric field, illustrating a rapid transition in the dominant energy contribution from the quantum confinement effect to the QCSE. Regarding the model Hamiltonian approach derived HRE  $\alpha_R$  given in Eq. (1),  $\alpha_R \simeq 2eCU E_x / \Delta$  when  $E_x < E_x^{\text{sat}}$ , consistent with what we have observed a linearly field-dependent HRE  $\alpha_R$  for  $E_x < 5$  kV/cm (Fig. 1 (a)). Whereas, when  $E_x > E_x^{\text{sat}}$  the QCSE is predominant in the  $\Delta(h0-h1)$  and thus  $\alpha_R \simeq C$  regarding Eq. (1), which explains the emergence of the

saturation of the atomistic pseudopotential method predicted HRE  $\alpha_R$  at  $E_x > 5$  kV/cm (Fig. 1 (a)).

Under a fixed electric field but varying the nanowire radius, the quantum confinement effect will be the primary factor in the  $h0$ - $h1$  splitting when nanowire is thin enough, whereas, the QCSE is always the leading factor at extremely wide nanowires. Fig. 2(c) shows that, as increasing the nanowire radius,  $\Delta(h0 - h1)$  undergoes a change from a steep reduction to a radius-independence for nanowires under a constant electric field  $E_x = 30$  kV/cm. This change indicates a transition in the dominant energy contribution from the quantum confinement effect at thin nanowires ( $R < 5$  nm) to the QCSE at wide nanowires ( $R > 5$  nm). Regarding Eq. (1),  $\alpha_R \simeq 2eCUE_x/\Delta \propto R^2$  for  $R < 5$  nm and  $\alpha_R \simeq C \propto 1/R$  for  $R > 5$  nm, consistent with the atomistic pseudopotential method prediction that  $\alpha_R \propto R^{2.3}$  for  $R < 5$  nm, and  $\alpha_R \propto 1/R^{0.4}$  for  $R > 5$  nm, as shown in Fig. 1 (b). Therefore, we ascribe the abnormal field- and radius-dependences of HRE  $\alpha_R$  in nanowires to the competition between the quantum confinement effect and electric field-induced QCSE on the  $h0 - h1$  splitting. We also note in Figs. 2(b) and 2(c) that, in the QCSE dominant scenario, the validity of the two-band approximation used in the model Hamiltonian approach is doubtful, regarding the first two subbands  $h0$  and  $h1$  are not well separated in energy from the next excited subband  $h2$ .

**Possible device implications of the theoretical work.** Like the drain-current saturation is an essential requirement in electronic field-effect transistors, the saturation of the electrically controlled Rashba effect is essential for practical applications of spintronic devices. The QCSE induced saturation of the HRE under the applied electric field can remarkably improve the scalability of semiconductor spintronic devices that rely on the Rashba effect, considering they can operate in the saturated region being robust against the fluctuations in applied electric fields. In conjunction with a huge HRE  $r_{ss}$  ( $\sim 300$  times larger than the ERE counterpart), which quantifies an ultrafast electrical response of the Rashba effect, the emergence of the rapid saturation of the HRE [reflected as the raising of the Rashba effect over just a narrow range of the electric field is in fact an advantage of the current proposition, since it could lead to the realization of an ultrafast switch of the Rashba field from zero to a saturation value using only a small gate voltage](#) [4, 8, 16]. Combining with the suppression of the D'yakonov-Perel' (DP) spin relaxation in nanowires [29–31] and remarkable reduction of hole spin-nuclear interaction [12], the unique HRE properties we have presented establish

1D hole nanowires to be an attractive platform for semiconductor spintronics applications [1, 2, 8]. Specifically, in Si nanowires the HRE  $\alpha_R^{\text{sat}}$  exceeds 100 meVÅ over a wide range of nanowire sizes, overcoming the major challenge of advanced Si spintronics owing to weak spin-orbit interaction in Si [6], and is insusceptible to fluctuations in nanowire sizes, making Si nanowires promising for the realization of scalable CMOS-compatible spintronics devices [2, 7].

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  - [26] (), since the Dresselhaus effect for 1D nanowires made of zinc-blende semiconductors vanishes by symmetry [17] for the (001)- and (111)-directions, any spin splitting we find upon application of an electric field perpendicular to the nanowire is fully a consequence of the Rashba effect arising from the breaking of the structural inversion symmetry.

- [27] (), the strength of the electron Rashba depends on superstructure bandgap:  $\alpha_R = aeP^2E_x[1/E_g(R)^2 - 1/(E_g(R) + \Delta_{\text{so}})^2]/3$  [13], where  $e$  is electron charge,  $a$  the adjustable parameter used to take into account all factors missed in classical Hamiltonian approach, InAs spin-orbit splitting  $\Delta_{\text{so}} = 0.38$  eV, InAs Kane's momentum matrix element  $P^2/2m = 21.5$  eV, and  $E_g(R)$  the nanowire bandgap. The predicted  $E_g(R)$  of InAs nanowires under  $E_x = 30$  kV/cm is described using  $E_g(R) = E_g^b + \beta/R^\gamma$ , where  $E_g^b = 0.417$  eV is bulk InAs bandgap,  $\beta = 2.8$ , and  $\gamma = 1.6$ .
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