Supporting Information for the manuscript

Revised electronic structure, Raman and IR studies of AB_2H_2 and *ABC*H (*A*=Sr, Ba; *B*= Al, Ga; *C* =Si, Ge) phases

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Table S1. The calculated equilibrium structural parameters (*a* and *c* are in Å) for the AB_2H_2 (*A* = Sr, Ba; *B* = Al, Ga) phases.

Compound	Cell parameters	Positional parameters
$SrAl_2H_2$	*a* = 4.5471 *c*= 4.7102	Sr(1*a*): 0, 0, 0 Al(2*d*): 1/3, 2/3, 0.4598 H(2*d*): 1/3, 2/3, 0.0955
$SrGa_2H_2$	*a* =4.4479 *c* = 4.7057	Sr(1*a*): 0, 0, 0 Ga(2*d*): 1/3, 2/3, 0.4628 H(2*d*): 1/3, 2/3, 0.1013
$BaAl_2H_2$	*a* = 4.6904 *c* = 4.9190	Ba(1*a*): 0, 0, 0 Al(2*d*): 1/3, 2/3, 0.4616 H(2*d*): 1/3, 2/3, 0.1259
$BaGa_2H_2$	*a* =4.5695 *c* = 4.9089	Ba(1*a*): 0, 0, 0 Ga(2*d*): 1/3, 2/3, 0.4688 H(2*d*): 1/3, 2/3, 0.1232

Table S2 The calculated equilibrium structural parameters (*a* and *c* are in Å) for the *ABC*H (*A* = Sr, Ba; *B* = Al, Ga; *C* = Si, Ge) phases.

Compound	Cell parameters	Positional parameters
SrAlSiH	*a*= 4.2971 *c*= 4.8902	Sr(1*a*): 0, 0, 0 Al(1*c*): 2/3, 1/3, 0.5383 Si(1*b*): 1/3, 2/3, 0.4465 H(1*c*): 2/3, 1/3, 0.8970
SrAlGeH	*a* =4.2683 *c* = 4.9131	Sr(1*a*): 0, 0, 0 Al(1*c*): 2/3, 1/3, 0.5450 Ge(1*b*): 1/3, 2/3, 0.4368 H(1*c*): 2/3, 1/3, 0.8929
SrGaSiH	*a* = 4.1943 *c* = 4.9483	Sr(1*a*): 0, 0, 0 Ga(1*c*): 2/3, 1/3, 0.5422 Si(1*b*): 1/3, 2/3, 0.4391 H(1*c*): 2/3, 1/3, 0.9000
SrGaGeH	*a* =4.2722 *c* = 4.9425	Sr(1*a*): 0, 0, 0 Ga(1*c*): 2/3, 1/3, 0.5495 Ge(1*b*): 1/3, 2/3, 0.4257 H(1*c*): 2/3, 1/3, 0.9052
BaAlSiH	*a* = 4.4004 *c* = 5.1958	Ba(1*a*): 0, 0, 0 Al(1*c*): 2/3, 1/3, 0.5373 Si(1*b*): 1/3, 2/3, 0.4568 H(1*c*): 2/3, 1/3, 0.8637
BaAlGeH	*a* =4.3901 *c* = 5.1942	Ba(1*a*): 0, 0, 0 Al(1*c*): 2/3, 1/3, 0.5370 Ge(1*b*): 1/3, 2/3, 0.4512 H(1*c*): 2/3, 1/3, 0.8708
BaGaSiH	*a* =4.3218 *c* = 5.1903	Ba(1*a*): 0, 0, 0 Ga(1*c*): 2/3, 1/3, 0.5375 Si(1*b*): 1/3, 2/3, 0.4485 H(1*c*): 2/3, 1/3, 0.8744
BaGaGeH	*a* =4.4040 *c* = 5.1557	Ba(1*a*): 0, 0, 0 Ga(1*c*): 2/3, 1/3, 0.5424 Ge(1*b*): 1/3, 2/3, 0.4380 H(1*c*): 2/3, 1/3, 0.8799

One can download the structure files (in cif format), simulated Raman and IR spectrum (both frequency as well as intensity) for these phases from our DFTBD (http://folk.uio.no/ponniahv/Database/) web site.

Table S3 The calculated interatomic distance in AB_2H_2 and $ABCH$ (A = Sr, Ba; B = Al, Ga; C = Si, Ge) phases. The corresponding experimental values are given in the parenthesis.

Compound	*B*-H (Å)	*B*-*B*/*B*-*C* (Å)	*A*-H (Å)
$SrAl_2H_2$	1.716 (1.706)[a]	2.650 (2.641)[a]	2.664 (2.653)[a]
$SrGa_2H_2$	1.701 (1.686)[b]	2.592 (2.557)[b]	2.601 (2.585)[b]
$BaAl_2H_2$	1.703	2.683	2.716
$BaGa_2H_2$	1.683 (1.689)[b]	2.656 (2.633)[b]	2.710 (2.683)[b]
SrAlSiH	1.754 (1.768)[c]	2.521(2.498)[c]	2.532 (2.477)[c]
SrAlGeH	1.709 (1.740)[b]	2.521 (2.488)[b]	2.520 (2.513)[b]
SrGaSiH	1.771 (1.769)[d]	2.475 (2.474)[d]	2.472 (2.466)[d]
SrGaGeH	1.758 (1.725)[d]	2.541 (2.508)[d]	2.511 (2.482)[d]
BaAlSiH	1.696 (1.733)[e]	2.575 (2.528)[e]	2.472 (2.581)[e]
BaAlGeH	1.734 (1.724)[b]	2.574 (2.54)[b]	2.622 (2.598)[b]
BaGaSiH	1.749 (1.758)[d]	2.538 (2.525)[d]	2.579 (2.568)[d]
BaGaGeH	1.741 (1.711)[d]	2.599 (2.555)[d]	2.617 (2.588)[d]

. [a]From ref.[3]; [b]From ref. [24]; [c]From ref.[2]; [d]From ref.[4]; [e]From ref.[25]