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Supporting Information

Critical Role of Dynamic Flexibility in Ge-Containing Zeolites: Impact on Diffusion

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A. Rabdel Ruiz-Salvador*^[a]

chem_201600983_sm_miscellaneous_information.pdf
chem_201600983_sm_s0_Si_ITQ29.avi
chem_201600983_sm_s1_SiGe_ITQ29.avi
chem_201600983_sm_s2_SiGe_ITQ29.avi
chem_201600983_sm_s3_SiGe_ITQ29.avi

Supporting Information

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- Crystallographic data of the Si-ITQ-29 (S0) and SiGe-ITQ-29 (S1, S2 and S3) structures used in this work, given as CIF format.
- Arrhenius fit of the diffusion coefficients obtained at different temperatures for Si-ITQ-29 and SiGe-ITQ-29 frameworks
- Movies coming from ab-initio Molecular Dynamics simulations (AIMD) performed for Si-ITQ-29 and SiGe-ITQ-29 frameworks. External AVI files:
 - s0_Si_ITQ29.avi,
 - s1_SiGe_ITQ29.avi,
 - s2_SiGe_ITQ29.avi and
 - s3_SiGe_ITQ29.avi

Crystallographic data of modeled S0 (Si-ITQ-29)

data_s0

_audit_creation_date 2015-07-30
_audit_creation_method 'VASP code'
_audit_author_name 'A. Rabdel Ruiz Salvador'

_citation_author_name 'Juan José Gutiérrez-Sevillano, Sofía Calero, Said Hamad, Salvador R. G. Balestra, Ricardo Grau-Crespo, Fernando Rey, Susana Valencia, Miguel Palomino and A. Rabdel Ruiz-Salvador'

_citation_title 'Critical role of dynamic flexibility in Ge-containing zeolites: impact on diffusion'

_symmetry_space_group_name_H-M 'P1'

_symmetry_Int_Tables_number 1

_symmetry_cell_setting triclinic

loop_

_symmetry_equiv_pos_as_xyz

x,y,z

_cell_length_a 11.9168

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_cell_angle_gamma 90.0000

loop_

_atom_site_label

_atom_site_type_symbol

_atom_site_fract_x

_atom_site_fract_y

_atom_site_fract_z

_atom_site_U_iso_or_equiv

_atom_site_adp_type

_atom_site_occupancy

Si1	Si	0.00000	0.18307	0.36807	0.00000	Uiso	1.00
Si2	Si	0.00000	0.81693	0.36807	0.00000	Uiso	1.00
Si3	Si	0.00000	0.18307	0.63193	0.00000	Uiso	1.00
Si4	Si	0.36807	0.00000	0.81693	0.00000	Uiso	1.00
Si5	Si	0.18307	0.00000	0.63193	0.00000	Uiso	1.00
Si6	Si	0.18307	0.00000	0.36807	0.00000	Uiso	1.00
Si7	Si	0.81693	0.00000	0.36807	0.00000	Uiso	1.00
Si8	Si	0.00000	0.81693	0.63193	0.00000	Uiso	1.00
Si9	Si	0.36807	0.00000	0.18307	0.00000	Uiso	1.00
Si10	Si	0.63193	0.00000	0.18307	0.00000	Uiso	1.00
Si11	Si	0.63193	0.00000	0.81693	0.00000	Uiso	1.00
Si12	Si	0.18307	0.36807	0.00000	0.00000	Uiso	1.00
Si13	Si	0.81693	0.36807	0.00000	0.00000	Uiso	1.00
Si14	Si	0.18307	0.63193	0.00000	0.00000	Uiso	1.00
Si15	Si	0.81693	0.63193	0.00000	0.00000	Uiso	1.00
Si16	Si	0.81693	0.00000	0.63193	0.00000	Uiso	1.00
Si17	Si	0.00000	0.36807	0.81693	0.00000	Uiso	1.00

Si18	Si	0.00000	0.36807	0.18307	0.00000	Uiso	1.00
Si19	Si	0.00000	0.63193	0.81693	0.00000	Uiso	1.00
Si20	Si	0.00000	0.63193	0.18307	0.00000	Uiso	1.00
Si21	Si	0.36807	0.18307	0.00000	0.00000	Uiso	1.00
Si22	Si	0.36807	0.81693	0.00000	0.00000	Uiso	1.00
Si23	Si	0.63193	0.18307	0.00000	0.00000	Uiso	1.00
Si24	Si	0.63193	0.81693	0.00000	0.00000	Uiso	1.00
O25	O	0.00000	0.21444	0.50000	0.00000	Uiso	1.00
O26	O	0.00000	0.78556	0.50000	0.00000	Uiso	1.00
O27	O	0.50000	0.00000	0.21444	0.00000	Uiso	1.00
O28	O	0.50000	0.00000	0.78556	0.00000	Uiso	1.00
O29	O	0.21444	0.50000	0.00000	0.00000	Uiso	1.00
O30	O	0.78556	0.50000	0.00000	0.00000	Uiso	1.00
O31	O	0.21444	0.00000	0.50000	0.00000	Uiso	1.00
O32	O	0.78556	0.00000	0.50000	0.00000	Uiso	1.00
O33	O	0.00000	0.50000	0.78556	0.00000	Uiso	1.00
O34	O	0.00000	0.50000	0.21444	0.00000	Uiso	1.00
O35	O	0.50000	0.21444	0.00000	0.00000	Uiso	1.00
O36	O	0.50000	0.78556	0.00000	0.00000	Uiso	1.00
O37	O	0.11160	0.11160	0.33664	0.00000	Uiso	1.00
O38	O	0.88840	0.88840	0.33664	0.00000	Uiso	1.00
O39	O	0.88840	0.11160	0.66336	0.00000	Uiso	1.00
O40	O	0.11160	0.88840	0.66336	0.00000	Uiso	1.00
O41	O	0.33664	0.11160	0.11160	0.00000	Uiso	1.00
O42	O	0.33664	0.88840	0.88840	0.00000	Uiso	1.00
O43	O	0.66336	0.88840	0.11160	0.00000	Uiso	1.00
O44	O	0.66336	0.11160	0.88840	0.00000	Uiso	1.00
O45	O	0.11160	0.33664	0.11160	0.00000	Uiso	1.00
O46	O	0.88840	0.33664	0.88840	0.00000	Uiso	1.00
O47	O	0.11160	0.66336	0.88840	0.00000	Uiso	1.00
O48	O	0.88840	0.66336	0.11160	0.00000	Uiso	1.00
O49	O	0.11160	0.11160	0.66336	0.00000	Uiso	1.00
O50	O	0.88840	0.88840	0.66336	0.00000	Uiso	1.00
O51	O	0.11160	0.88840	0.33664	0.00000	Uiso	1.00
O52	O	0.88840	0.11160	0.33664	0.00000	Uiso	1.00
O53	O	0.11160	0.33664	0.88840	0.00000	Uiso	1.00
O54	O	0.88840	0.33664	0.11160	0.00000	Uiso	1.00
O55	O	0.88840	0.66336	0.88840	0.00000	Uiso	1.00
O56	O	0.11160	0.66336	0.11160	0.00000	Uiso	1.00
O57	O	0.33664	0.11160	0.88840	0.00000	Uiso	1.00
O58	O	0.33664	0.88840	0.11160	0.00000	Uiso	1.00
O59	O	0.66336	0.11160	0.11160	0.00000	Uiso	1.00
O60	O	0.66336	0.88840	0.88840	0.00000	Uiso	1.00
O61	O	0.00000	0.29859	0.29859	0.00000	Uiso	1.00
O62	O	0.00000	0.70141	0.29859	0.00000	Uiso	1.00
O63	O	0.00000	0.29859	0.70141	0.00000	Uiso	1.00
O64	O	0.00000	0.70141	0.70141	0.00000	Uiso	1.00
O65	O	0.29859	0.00000	0.29859	0.00000	Uiso	1.00
O66	O	0.29859	0.00000	0.70141	0.00000	Uiso	1.00
O67	O	0.70141	0.00000	0.29859	0.00000	Uiso	1.00

O68	O	0.70141	0.00000	0.70141	0.00000	Uiso	1.00
O69	O	0.29859	0.29859	0.00000	0.00000	Uiso	1.00
O70	O	0.70141	0.29859	0.00000	0.00000	Uiso	1.00
O71	O	0.29859	0.70141	0.00000	0.00000	Uiso	1.00
O72	O	0.70141	0.70141	0.00000	0.00000	Uiso	1.00

Crystallographic data of modeled S1 (SiGe-ITQ-29)

data_s1

_audit_creation_date 2015-07-30
_audit_creation_method 'VASP code'
_audit_author_name 'A. Rabdel Ruiz Salvador'

_citation_author_name 'Juan José Gutiérrez-Sevillano, Sofía Calero, Said Hamad, Salvador R. G. Balestra, Ricardo Grau-Crespo, Fernando Rey, Susana Valencia, Miguel Palomino and A. Rabdel Ruiz-Salvador'

_citation_title 'Critical role of dynamic flexibility in Ge-containing zeolites: impact on diffusion'

_symmetry_space_group_name_H-M 'P1'

_symmetry_Int_Tables_number 1

_symmetry_cell_setting triclinic

loop_

_symmetry_equiv_pos_as_xyz

x,y,z

_cell_length_a 12.0992

_cell_length_b 12.0992

_cell_length_c 12.0992

_cell_angle_alpha 90.0000

_cell_angle_beta 90.0000

_cell_angle_gamma 90.0000

loop_

_atom_site_label

_atom_site_type_symbol

_atom_site_fract_x

_atom_site_fract_y

_atom_site_fract_z

_atom_site_U_iso_or_equiv

_atom_site_adp_type

_atom_site_occupancy

Ge1	Ge	0.00141	0.18748	0.35883	0.00000	Uiso	1.00
Ge2	Ge	0.00126	0.80624	0.36711	0.00000	Uiso	1.00
Ge3	Ge	0.00483	0.18646	0.64033	0.00000	Uiso	1.00
Ge4	Ge	0.37293	0.99819	0.81564	0.00000	Uiso	1.00
Ge5	Ge	0.18194	0.99827	0.63760	0.00000	Uiso	1.00
Ge6	Ge	0.18040	0.99915	0.35021	0.00000	Uiso	1.00
Ge7	Ge	0.80805	0.99983	0.36927	0.00000	Uiso	1.00
Si8	Si	0.00491	0.81359	0.63828	0.00000	Uiso	1.00
Si9	Si	0.36692	0.00117	0.17286	0.00000	Uiso	1.00
Si10	Si	0.63123	0.00010	0.17748	0.00000	Uiso	1.00
Si11	Si	0.64154	0.99726	0.82630	0.00000	Uiso	1.00
Si12	Si	0.18260	0.36814	0.00022	0.00000	Uiso	1.00
Si13	Si	0.81581	0.36788	0.00194	0.00000	Uiso	1.00
Si14	Si	0.18122	0.63349	0.00357	0.00000	Uiso	1.00
Si15	Si	0.81465	0.63208	0.00584	0.00000	Uiso	1.00
Si16	Si	0.82021	0.00007	0.63721	0.00000	Uiso	1.00
Si17	Si	0.99962	0.37441	0.82280	0.00000	Uiso	1.00

Si18	Si	0.99948	0.36659	0.17310	0.00000	Uiso	1.00
Si19	Si	0.99795	0.63570	0.82644	0.00000	Uiso	1.00
Si20	Si	0.99833	0.63138	0.17677	0.00000	Uiso	1.00
Si21	Si	0.36726	0.18540	0.99802	0.00000	Uiso	1.00
Si22	Si	0.36652	0.81422	0.00158	0.00000	Uiso	1.00
Si23	Si	0.63375	0.18245	0.00169	0.00000	Uiso	1.00
Si24	Si	0.63205	0.81530	0.00640	0.00000	Uiso	1.00
O25	O	0.02534	0.21522	0.49932	0.00000	Uiso	1.00
O26	O	0.01329	0.77870	0.50905	0.00000	Uiso	1.00
O27	O	0.49869	0.00035	0.18766	0.00000	Uiso	1.00
O28	O	0.51414	0.99984	0.78783	0.00000	Uiso	1.00
O29	O	0.20550	0.50091	0.00590	0.00000	Uiso	1.00
O30	O	0.78908	0.49983	0.00878	0.00000	Uiso	1.00
O31	O	0.17130	0.01819	0.49400	0.00000	Uiso	1.00
O32	O	0.77676	0.00179	0.51062	0.00000	Uiso	1.00
O33	O	0.00038	0.50548	0.79872	0.00000	Uiso	1.00
O34	O	0.99982	0.49891	0.18324	0.00000	Uiso	1.00
O35	O	0.50070	0.20631	0.00050	0.00000	Uiso	1.00
O36	O	0.49930	0.79161	0.00693	0.00000	Uiso	1.00
O37	O	0.10976	0.11374	0.29244	0.00000	Uiso	1.00
O38	O	0.87856	0.87745	0.33028	0.00000	Uiso	1.00
O39	O	0.88126	0.11547	0.66921	0.00000	Uiso	1.00
O40	O	0.11859	0.87376	0.67909	0.00000	Uiso	1.00
O41	O	0.33094	0.11178	0.10506	0.00000	Uiso	1.00
O42	O	0.33304	0.87697	0.88658	0.00000	Uiso	1.00
O43	O	0.66859	0.88721	0.11430	0.00000	Uiso	1.00
O44	O	0.66975	0.10980	0.89426	0.00000	Uiso	1.00
O45	O	0.11040	0.32847	0.10690	0.00000	Uiso	1.00
O46	O	0.88864	0.34175	0.89175	0.00000	Uiso	1.00
O47	O	0.11038	0.66702	0.89380	0.00000	Uiso	1.00
O48	O	0.88588	0.67008	0.11370	0.00000	Uiso	1.00
O49	O	0.11805	0.11465	0.70019	0.00000	Uiso	1.00
O50	O	0.90051	0.89497	0.65766	0.00000	Uiso	1.00
O51	O	0.12063	0.87118	0.31182	0.00000	Uiso	1.00
O52	O	0.87331	0.12380	0.32741	0.00000	Uiso	1.00
O53	O	0.11158	0.33973	0.88927	0.00000	Uiso	1.00
O54	O	0.88749	0.32845	0.10892	0.00000	Uiso	1.00
O55	O	0.88680	0.66366	0.89681	0.00000	Uiso	1.00
O56	O	0.10914	0.67109	0.11126	0.00000	Uiso	1.00
O57	O	0.33161	0.11991	0.88505	0.00000	Uiso	1.00
O58	O	0.32913	0.89052	0.10624	0.00000	Uiso	1.00
O59	O	0.66817	0.11154	0.11128	0.00000	Uiso	1.00
O60	O	0.66623	0.88672	0.89815	0.00000	Uiso	1.00
O61	O	0.99900	0.31869	0.29788	0.00000	Uiso	1.00
O62	O	0.99700	0.67667	0.30281	0.00000	Uiso	1.00
O63	O	0.99703	0.31650	0.70243	0.00000	Uiso	1.00
O64	O	0.99210	0.70309	0.71146	0.00000	Uiso	1.00
O65	O	0.31534	0.00108	0.29722	0.00000	Uiso	1.00
O66	O	0.32094	0.99456	0.67924	0.00000	Uiso	1.00
O67	O	0.68006	0.99964	0.30195	0.00000	Uiso	1.00

O68	O	0.71368	0.99023	0.71525	0.00000	Uiso	1.00
O69	O	0.29958	0.30155	0.99943	0.00000	Uiso	1.00
O70	O	0.70059	0.29885	0.99962	0.00000	Uiso	1.00
O71	O	0.29871	0.69854	0.00445	0.00000	Uiso	1.00
O72	O	0.69837	0.69890	0.00480	0.00000	Uiso	1.00

Crystallographic data of modeled S2 (SiGe-ITQ-29)

data_s2

_audit_creation_date 2015-07-30
_audit_creation_method 'VASP code'
_audit_author_name 'A. Rabdel Ruiz Salvador'

_citation_author_name 'Juan José Gutiérrez-Sevillano, Sofía Calero, Said Hamad, Salvador R. G. Balestra, Ricardo Grau-Crespo, Fernando Rey, Susana Valencia, Miguel Palomino and A. Rabdel Ruiz-Salvador'

_citation_title 'Critical role of dynamic flexibility in Ge-containing zeolites: impact on diffusion'

_symmetry_space_group_name_H-M 'P1'

_symmetry_Int_Tables_number 1

_symmetry_cell_setting triclinic

loop_

_symmetry_equiv_pos_as_xyz

x,y,z

_cell_length_a 12.0384

_cell_length_b 12.0384

_cell_length_c 12.0384

_cell_angle_alpha 90.0000

_cell_angle_beta 90.0000

_cell_angle_gamma 90.0000

loop_

_atom_site_label

_atom_site_type_symbol

_atom_site_fract_x

_atom_site_fract_y

_atom_site_fract_z

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_atom_site_adp_type

_atom_site_occupancy

Ge1	Ge	0.00067	0.18092	0.36364	0.00000	Uiso	1.00
Ge2	Ge	0.99963	0.81625	0.36901	0.00000	Uiso	1.00
Ge3	Ge	0.36839	0.00223	0.81399	0.00000	Uiso	1.00
Ge4	Ge	0.18007	0.36690	0.00122	0.00000	Uiso	1.00
Ge5	Ge	0.17855	0.00096	0.63470	0.00000	Uiso	1.00
Ge6	Ge	0.99909	0.63761	0.17856	0.00000	Uiso	1.00
Ge7	Ge	0.36787	0.18423	0.00123	0.00000	Uiso	1.00
Si8	Si	0.99977	0.18453	0.63724	0.00000	Uiso	1.00
Si9	Si	0.99977	0.81812	0.64315	0.00000	Uiso	1.00
Si10	Si	0.36769	0.99710	0.18269	0.00000	Uiso	1.00
Si11	Si	0.63355	0.99711	0.18144	0.00000	Uiso	1.00
Si12	Si	0.64378	0.00096	0.82191	0.00000	Uiso	1.00
Si13	Si	0.81691	0.36838	0.00226	0.00000	Uiso	1.00
Si14	Si	0.17921	0.64420	0.99982	0.00000	Uiso	1.00
Si15	Si	0.81142	0.63120	0.00201	0.00000	Uiso	1.00
Si16	Si	0.81830	0.99948	0.63217	0.00000	Uiso	1.00
Si17	Si	0.18099	0.99811	0.35522	0.00000	Uiso	1.00

Si18	Si	0.80979	0.99679	0.36811	0.00000	Uiso	1.00
Si19	Si	0.99887	0.36909	0.81636	0.00000	Uiso	1.00
Si20	Si	0.99964	0.36120	0.17801	0.00000	Uiso	1.00
Si21	Si	0.99947	0.63220	0.82087	0.00000	Uiso	1.00
Si22	Si	0.36779	0.81687	0.99915	0.00000	Uiso	1.00
Si23	Si	0.64454	0.17639	0.00144	0.00000	Uiso	1.00
Si24	Si	0.63303	0.81720	0.99897	0.00000	Uiso	1.00
O25	O	0.01256	0.20849	0.50584	0.00000	Uiso	1.00
O26	O	0.01428	0.79637	0.51187	0.00000	Uiso	1.00
O27	O	0.50058	0.00212	0.20162	0.00000	Uiso	1.00
O28	O	0.51224	0.01076	0.79906	0.00000	Uiso	1.00
O29	O	0.19203	0.51140	0.01122	0.00000	Uiso	1.00
O30	O	0.78541	0.49921	0.00919	0.00000	Uiso	1.00
O31	O	0.18467	0.99855	0.48924	0.00000	Uiso	1.00
O32	O	0.78804	0.99767	0.50094	0.00000	Uiso	1.00
O33	O	0.00763	0.50108	0.79197	0.00000	Uiso	1.00
O34	O	0.01462	0.49372	0.18418	0.00000	Uiso	1.00
O35	O	0.51227	0.19667	0.99589	0.00000	Uiso	1.00
O36	O	0.50032	0.79453	0.99571	0.00000	Uiso	1.00
O37	O	0.11919	0.11134	0.31218	0.00000	Uiso	1.00
O38	O	0.87514	0.88374	0.33195	0.00000	Uiso	1.00
O39	O	0.89004	0.10980	0.66128	0.00000	Uiso	1.00
O40	O	0.10941	0.88361	0.68937	0.00000	Uiso	1.00
O41	O	0.32474	0.10922	0.11951	0.00000	Uiso	1.00
O42	O	0.32752	0.88268	0.88773	0.00000	Uiso	1.00
O43	O	0.66465	0.88514	0.11179	0.00000	Uiso	1.00
O44	O	0.68607	0.10798	0.89254	0.00000	Uiso	1.00
O45	O	0.10834	0.30876	0.11548	0.00000	Uiso	1.00
O46	O	0.88924	0.34422	0.89101	0.00000	Uiso	1.00
O47	O	0.11018	0.67284	0.88702	0.00000	Uiso	1.00
O48	O	0.87281	0.67526	0.11463	0.00000	Uiso	1.00
O49	O	0.11152	0.12218	0.68325	0.00000	Uiso	1.00
O50	O	0.88776	0.88926	0.66664	0.00000	Uiso	1.00
O51	O	0.11440	0.88769	0.31255	0.00000	Uiso	1.00
O52	O	0.87826	0.10745	0.33070	0.00000	Uiso	1.00
O53	O	0.11216	0.32606	0.87766	0.00000	Uiso	1.00
O54	O	0.88690	0.33027	0.11097	0.00000	Uiso	1.00
O55	O	0.88875	0.65633	0.89433	0.00000	Uiso	1.00
O56	O	0.11367	0.69534	0.10756	0.00000	Uiso	1.00
O57	O	0.31409	0.12316	0.87827	0.00000	Uiso	1.00
O58	O	0.33698	0.88714	0.11040	0.00000	Uiso	1.00
O59	O	0.67491	0.10641	0.11323	0.00000	Uiso	1.00
O60	O	0.67128	0.88787	0.89036	0.00000	Uiso	1.00
O61	O	0.99206	0.31285	0.30321	0.00000	Uiso	1.00
O62	O	0.99715	0.67932	0.31832	0.00000	Uiso	1.00
O63	O	0.98789	0.30234	0.70048	0.00000	Uiso	1.00
O64	O	0.99083	0.69999	0.70561	0.00000	Uiso	1.00
O65	O	0.30454	0.99312	0.30169	0.00000	Uiso	1.00
O66	O	0.31862	0.99708	0.67645	0.00000	Uiso	1.00
O67	O	0.69276	0.99598	0.30208	0.00000	Uiso	1.00

O68	O	0.70451	0.99988	0.70252	0.00000	Uiso	1.00
O69	O	0.31929	0.32206	0.00546	0.00000	Uiso	1.00
O70	O	0.70389	0.29658	0.00091	0.00000	Uiso	1.00
O71	O	0.30151	0.69998	0.99846	0.00000	Uiso	1.00
O72	O	0.69552	0.69845	0.99453	0.00000	Uiso	1.00

Crystallographic data of modeled S3 (SiGe-ITQ-29)

data_s3

_audit_creation_date 2015-07-30
_audit_creation_method 'VASP code'
_audit_author_name 'A. Rabdel Ruiz Salvador'

_citation_author_name 'Juan José Gutiérrez-Sevillano, Sofía Calero, Said Hamad, Salvador R. G. Balestra, Ricardo Grau-Crespo, Fernando Rey, Susana Valencia, Miguel Palomino and A. Rabdel Ruiz-Salvador'

_citation_title 'Critical role of dynamic flexibility in Ge-containing zeolites: impact on diffusion'

_symmetry_space_group_name_H-M 'P1'

_symmetry_Int_Tables_number 1

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x,y,z

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loop_

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_atom_site_fract_y

_atom_site_fract_z

_atom_site_U_iso_or_equiv

_atom_site_adp_type

_atom_site_occupancy

Ge1	Ge	0.99950	0.18074	0.35458	0.00000	Uiso	1.00
Ge2	Ge	0.99917	0.81483	0.36204	0.00000	Uiso	1.00
Ge3	Ge	0.00017	0.18290	0.63566	0.00000	Uiso	1.00
Ge4	Ge	0.99977	0.81660	0.63893	0.00000	Uiso	1.00
Ge5	Ge	0.18560	0.35743	0.00043	0.00000	Uiso	1.00
Ge6	Ge	0.18245	0.64325	0.99958	0.00000	Uiso	1.00
Ge7	Ge	0.99710	0.36349	0.82322	0.00000	Uiso	1.00
Si8	Si	0.36802	0.99871	0.18273	0.00000	Uiso	1.00
Si9	Si	0.36831	0.00187	0.81811	0.00000	Uiso	1.00
Si10	Si	0.63404	0.99895	0.18250	0.00000	Uiso	1.00
Si11	Si	0.63471	0.00225	0.81948	0.00000	Uiso	1.00
Si12	Si	0.80813	0.36818	0.99998	0.00000	Uiso	1.00
Si13	Si	0.81165	0.63257	0.00016	0.00000	Uiso	1.00
Si14	Si	0.18749	0.00098	0.63480	0.00000	Uiso	1.00
Si15	Si	0.81165	0.00214	0.63428	0.00000	Uiso	1.00
Si16	Si	0.18708	0.99941	0.36433	0.00000	Uiso	1.00
Si17	Si	0.81093	0.99967	0.36583	0.00000	Uiso	1.00

Si18	Si	0.99765	0.36719	0.17523	0.00000	Uiso	1.00
Si19	Si	0.99804	0.63947	0.82736	0.00000	Uiso	1.00
Si20	Si	0.99735	0.63301	0.17674	0.00000	Uiso	1.00
Si21	Si	0.37045	0.17577	0.00149	0.00000	Uiso	1.00
Si22	Si	0.37115	0.82325	0.99979	0.00000	Uiso	1.00
Si23	Si	0.63670	0.17729	0.00228	0.00000	Uiso	1.00
Si24	Si	0.63664	0.82245	0.00027	0.00000	Uiso	1.00
O25	O	0.00664	0.21271	0.49491	0.00000	Uiso	1.00
O26	O	0.00458	0.77377	0.50075	0.00000	Uiso	1.00
O27	O	0.50105	0.00012	0.20176	0.00000	Uiso	1.00
O28	O	0.50162	0.00310	0.79917	0.00000	Uiso	1.00
O29	O	0.21160	0.50053	0.99469	0.00000	Uiso	1.00
O30	O	0.78311	0.50065	0.99786	0.00000	Uiso	1.00
O31	O	0.20059	0.00249	0.49951	0.00000	Uiso	1.00
O32	O	0.79550	0.00415	0.50004	0.00000	Uiso	1.00
O33	O	0.01808	0.50703	0.82803	0.00000	Uiso	1.00
O34	O	0.01031	0.49997	0.18499	0.00000	Uiso	1.00
O35	O	0.50350	0.19060	0.00164	0.00000	Uiso	1.00
O36	O	0.50387	0.80422	0.99944	0.00000	Uiso	1.00
O37	O	0.12181	0.10895	0.31726	0.00000	Uiso	1.00
O38	O	0.87672	0.88755	0.32849	0.00000	Uiso	1.00
O39	O	0.87803	0.11273	0.67573	0.00000	Uiso	1.00
O40	O	0.12192	0.88916	0.67519	0.00000	Uiso	1.00
O41	O	0.33142	0.10790	0.11186	0.00000	Uiso	1.00
O42	O	0.33416	0.89189	0.88914	0.00000	Uiso	1.00
O43	O	0.67116	0.88899	0.11294	0.00000	Uiso	1.00
O44	O	0.67321	0.11194	0.88931	0.00000	Uiso	1.00
O45	O	0.10882	0.31537	0.11807	0.00000	Uiso	1.00
O46	O	0.86995	0.32781	0.88623	0.00000	Uiso	1.00
O47	O	0.10678	0.69613	0.88542	0.00000	Uiso	1.00
O48	O	0.88409	0.66289	0.10987	0.00000	Uiso	1.00
O49	O	0.12104	0.11133	0.67789	0.00000	Uiso	1.00
O50	O	0.87819	0.89079	0.67263	0.00000	Uiso	1.00
O51	O	0.12097	0.88751	0.32498	0.00000	Uiso	1.00
O52	O	0.87711	0.10851	0.31998	0.00000	Uiso	1.00
O53	O	0.11597	0.30091	0.88328	0.00000	Uiso	1.00
O54	O	0.88591	0.33764	0.10584	0.00000	Uiso	1.00
O55	O	0.88298	0.66827	0.89139	0.00000	Uiso	1.00
O56	O	0.10820	0.68500	0.11894	0.00000	Uiso	1.00
O57	O	0.33177	0.11153	0.88869	0.00000	Uiso	1.00
O58	O	0.33370	0.88860	0.11221	0.00000	Uiso	1.00
O59	O	0.67297	0.10831	0.11290	0.00000	Uiso	1.00
O60	O	0.67143	0.89225	0.88955	0.00000	Uiso	1.00
O61	O	0.98946	0.31419	0.29800	0.00000	Uiso	1.00
O62	O	0.99031	0.68382	0.30025	0.00000	Uiso	1.00
O63	O	0.99336	0.32066	0.68439	0.00000	Uiso	1.00
O64	O	0.99076	0.68603	0.70209	0.00000	Uiso	1.00
O65	O	0.30733	0.99795	0.30330	0.00000	Uiso	1.00
O66	O	0.30702	0.00093	0.69761	0.00000	Uiso	1.00
O67	O	0.69141	0.99835	0.30436	0.00000	Uiso	1.00

O68	O	0.69321	0.00148	0.69798	0.00000	Uiso	1.00
O69	O	0.31886	0.29980	0.00493	0.00000	Uiso	1.00
O70	O	0.69299	0.29939	0.00693	0.00000	Uiso	1.00
O71	O	0.31554	0.70108	0.99939	0.00000	Uiso	1.00
O72	O	0.69729	0.70260	0.00039	0.00000	Uiso	1.00

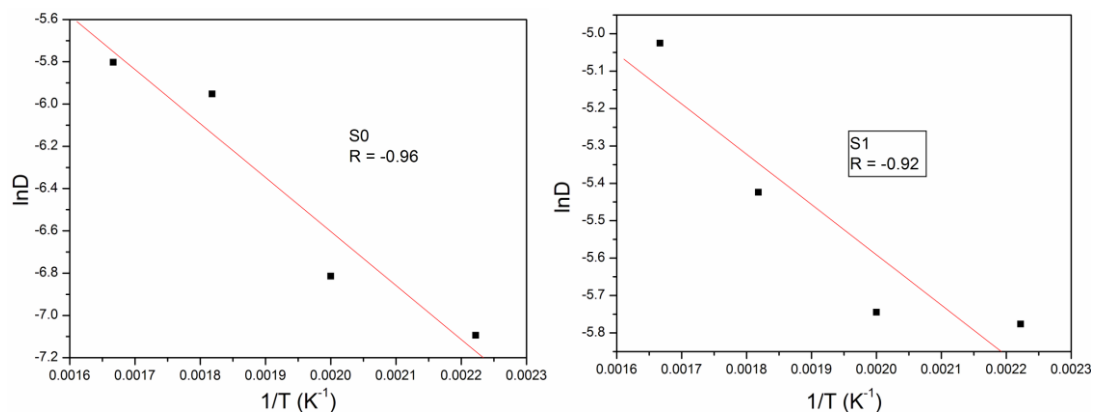


Figure S1. Arrhenius fit of the diffusion coefficients obtained at different temperatures for Si-ITQ-29 (top) and SiGe-ITQ-29 (bottom) frameworks.