CYCLOHEXASILANE: PHYSICAL PROPERTIES & NANOMATERIAL GROWTH

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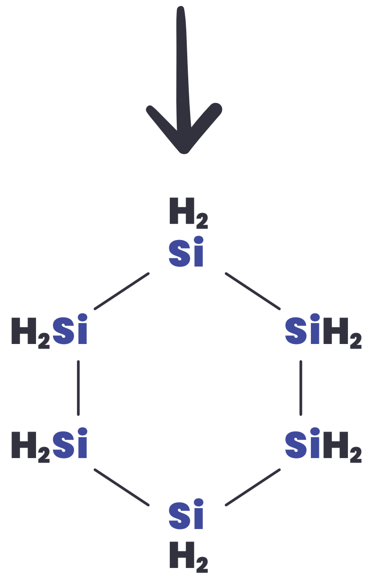
THE CORETEC GROUP
ENGINEERING SILICON TO IMPROVE LIFE

CYCLOHEXASILANE DETAILS

PROPERTY	VALUE
Melting Point	18 °C
Boiling Point	226 °C (80 °C @ 10 torr)
Density	0.97 g/cm^3
Stability	> 12 months
Purity	> 98%

Inexpensive raw commodity chemicals (e.g. $HSiCl_3$)
High atom economy, high yielding



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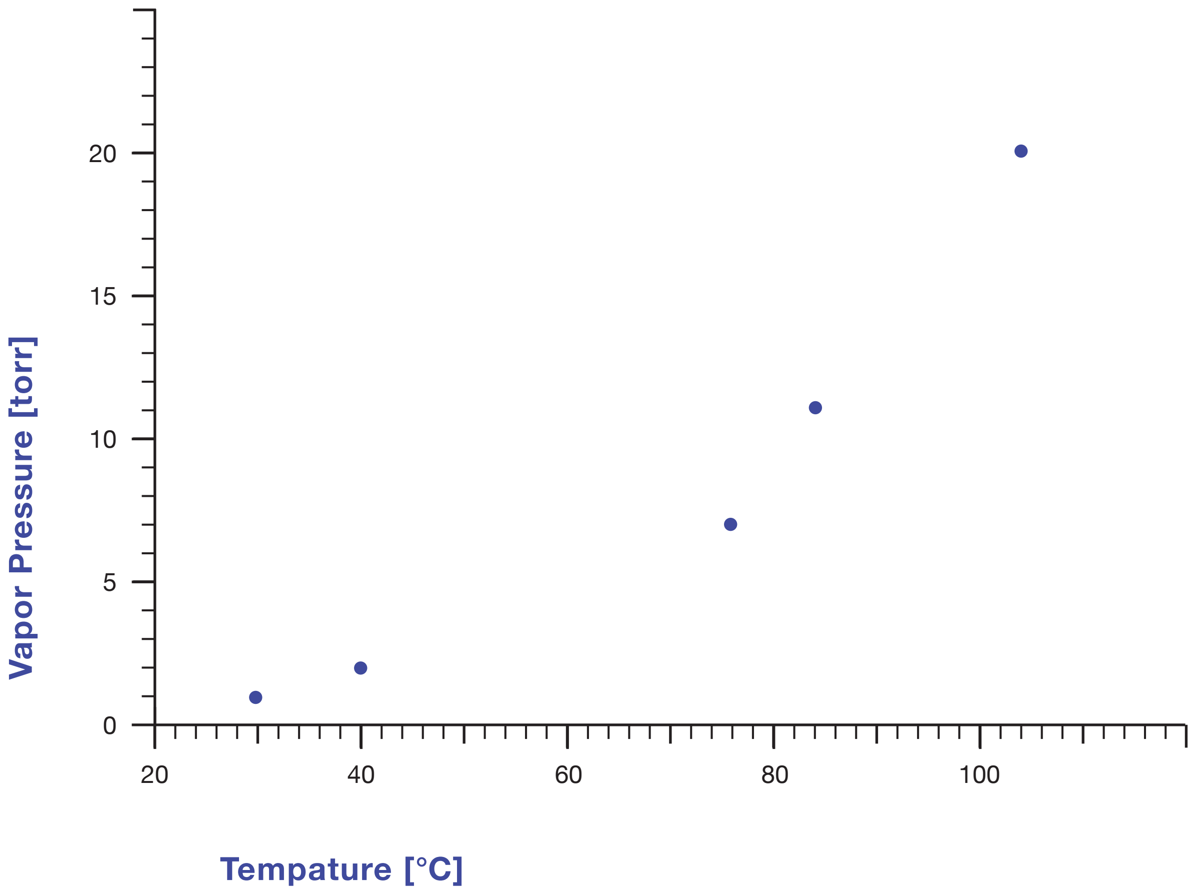
CYCLOHEXASILANE VAPOR PRESSURE AS A FUNCTION OF TEMPERATURE



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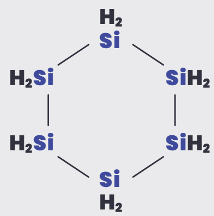
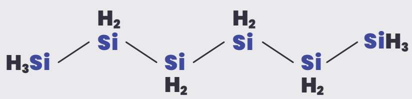
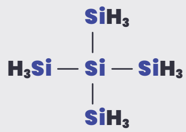
BOND ENTHALPY COMPARISON

CHEMICAL NAME	CHEMICAL STRUCTURE	Si-Si BOND (kj/mol)	Si-H BOND (kj/mol)
Cylohexasilane (CHS)		**262**	**343**
Hexasilane		277	354
neo-Pentasilane		268	357
Disilane	$H_3Si — SiH_3$	289	364
Monosilane	SiH_4	—	372

Lower BDE

Deposition: Lower T & Faster

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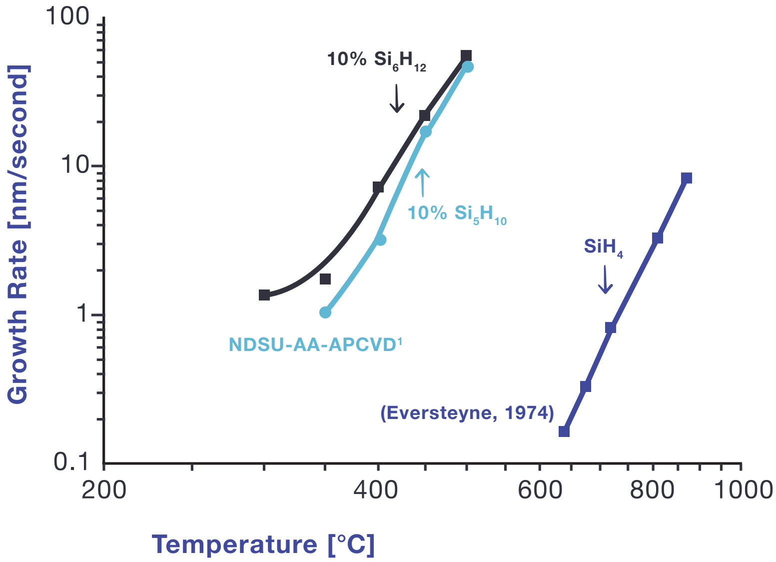
AEROSOL ASSISTED CVD OF SI THIN FILMS

AA-APCVD Characteristics:

- Aerosolized liquid precursor
- Atmospheric pressure
- Continuous and scalable (R2R)
- High deposition efficiency at low thermal budget

Liquid Precursor Formulations For:

- Intrinsic silicon
- n and p doped silicon
- Low K dielectrics (SiOCN)
- Si-C compositions
- SiNx



Sllane	E_a (eV)
SiH_4	1.6-2.5*
Si_2H_4	2.2*
Si_3H_8	1.63*
Si_4H_{10}	1.38*
Si_5H_{10}	0.34
Si_6H_{12}	0.30

Deposition rates and activation energies of hydrosilanes (Si_6H_{12} has lowest E_a of known silanes)

Comparison Of Si Film Deposition Techniques

	AA-APCVD w/ Si_6H_{12} (exp.)	LPCVD w/ SiH_4 (lit.)	PECVD w/ SiH_4 (lit.)
Growth rate (nm/sec)	~17 (un-optimized)	0.01 to 1	1–5
Precursors	Soluble Solids/Liquids	Pyrophoric/Toxic Gases	Pyrophoric/Toxic Gases
Temperature	300 – 500+ °C	500 – 1000 °C	25 – 450 °C
Photosensitivity	$10^3 – 10^4$ (a-Si:H)	$10^2 – 10^7$ (a-Si:H and c-Si)	$10^3 – 10^6$ (a-Si:H)
Si Dep. eff.	~40% (un-optimized)	up to ~100%	~15% (Established)

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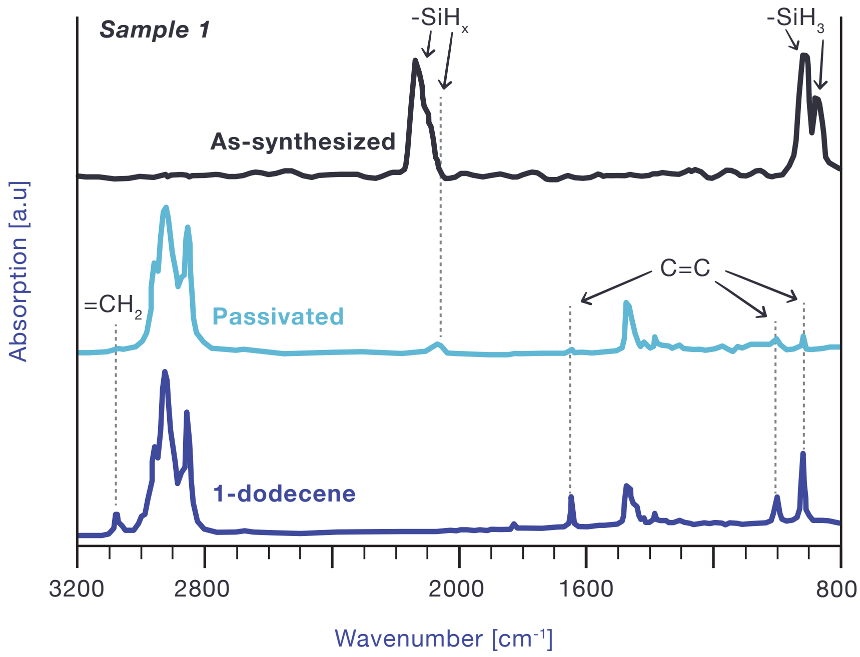
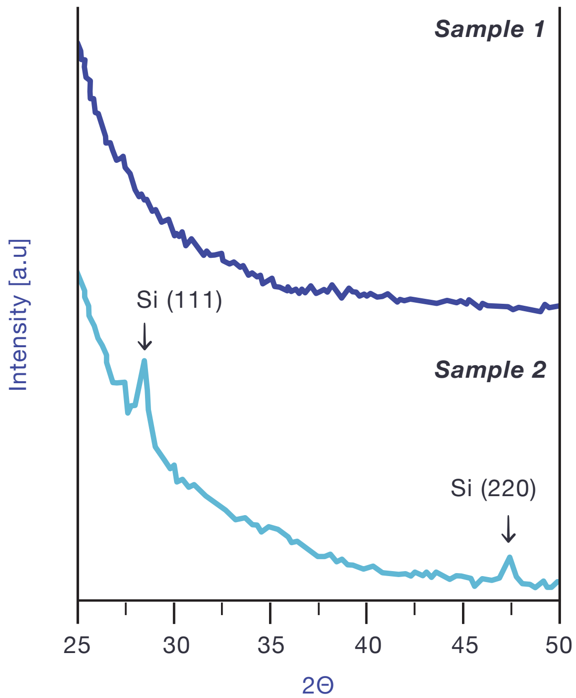
1. https://www.sciencedirect.com/science/article/abs/pii/S0040609015006112

CONTROL OF SURFACE CHEMISTRY & CRYSTALLINITY

FTIR indicates efficient hydrosilylation



Annealing at 400 °C:



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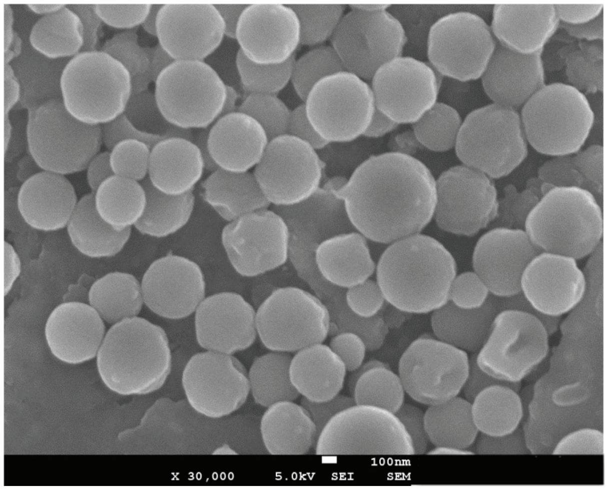
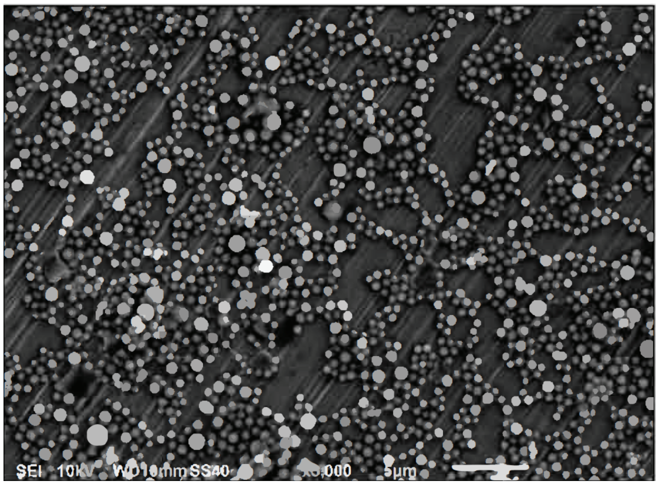
SOLUTION/EMULSION POLYMERIZATION

CHS spontaneously or inductively forms nano-sized domains in select liquid systems such as microemulsions which can be processed to generate silicon nanostructures.

Generation of these nanostructures is enabled by the ability to transform CHS into structurally robust polysilane colloids at RT using UV irradiation or chemical initiators.



SEM image of polysilane colloids generated by micro-emulsion polymerization of Si_6H_{12} using UV irradiation.



SEM image of a-Si colloids generated by micro-emulsion polymerization of Si_6H_{12} and heat treatment at 400 °C.

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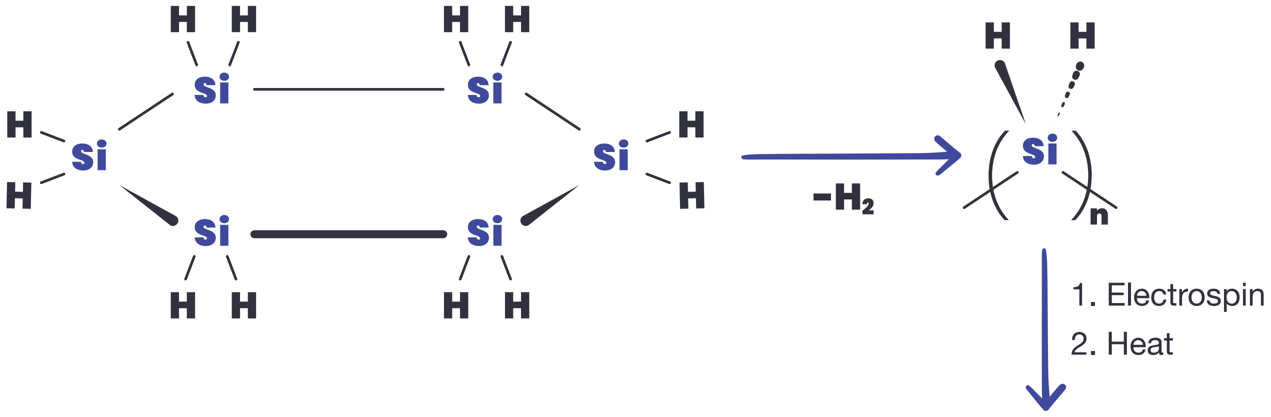
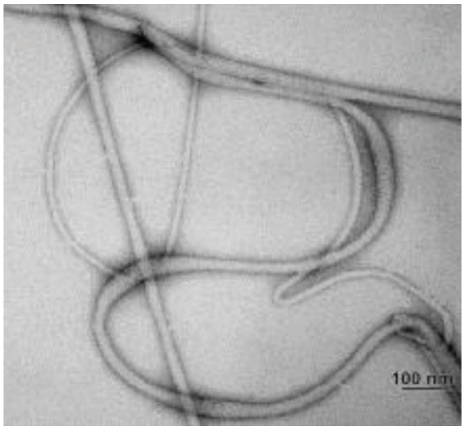
ELECTROSPUN SI NWS FROM CHS-BASED INKS

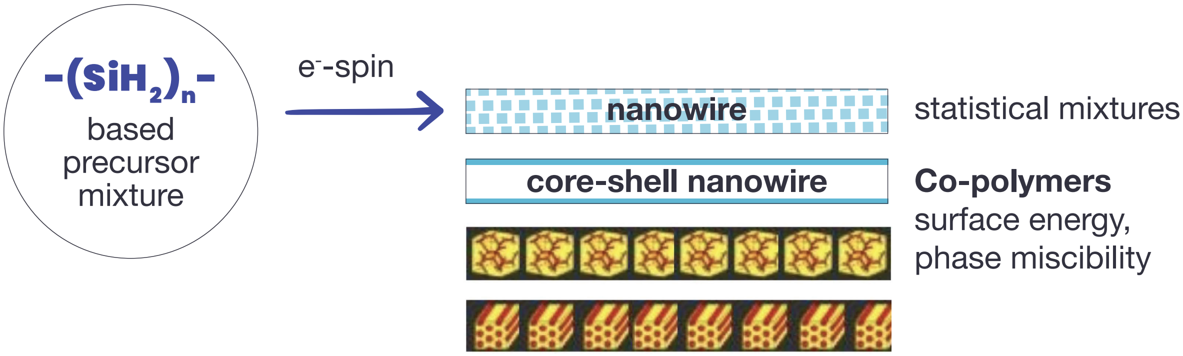




Si nanofibers as Li Ion Battery Anode

1. >10-fold increase in energy density compared to graphite
2. d<100 nm, amorphous structure
3. scalable process
4. low cycle loss

Potential for New Copolymer Physical Chemistry



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ADVANTAGES OF SI_6H_{12} AS A PECVD PRECURSOR

1. CHS molecule consists of **6 Si atoms which can be simultaneously** delivered into the PECVD chamber thus enabling higher deposition rate compared to traditional monosilane.

2. Our experiments have shown that good quality a-Si:H films can be fabricated. This finding allows to partially **eliminate a costly multistage purification process,** thus making CHS a more cost efficient precursor than traditional silanes.

3. CHS has a low vapor pressure at room temperature (0.3 torr), which makes all operations with this precursor much safer than similar operations with gaseous silanes.

4. CHS **does not require any dilution** when used (gaseous silanes are diluted with He). This characteristic significantly widens Si delivery and hydrogen dilution ranges.

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