Supplementary Information for:

Sulfur geochemical evidence for a high-energy impact lunar origin

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This file includes:

Figs. S1–S5
Table S1

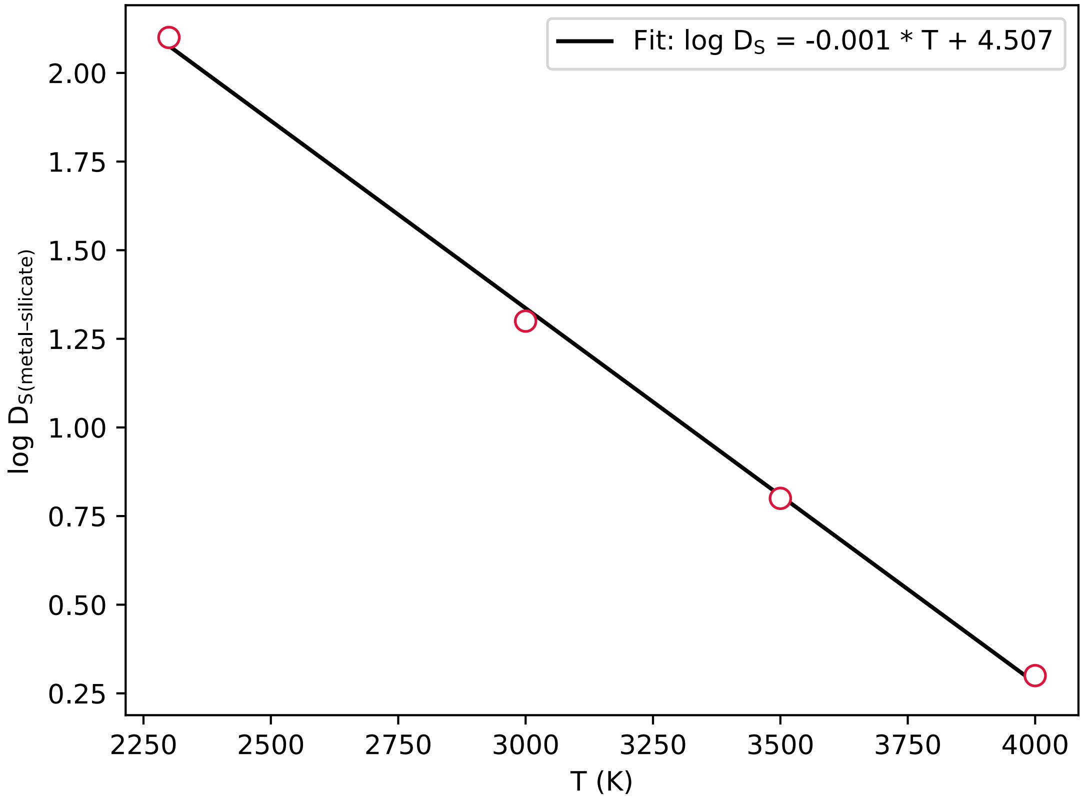

Fig. S1. Fitting equation for $D^{S}_{metal-silicate}$, the sulfur metal-silicate partition coefficient, as a function of temperature at lunar core-mantle boundary pressure (~4.5 GPa)[38]. Data are from sulfur metal-silicate partitioning studies[4] conducted across a range of temperatures.

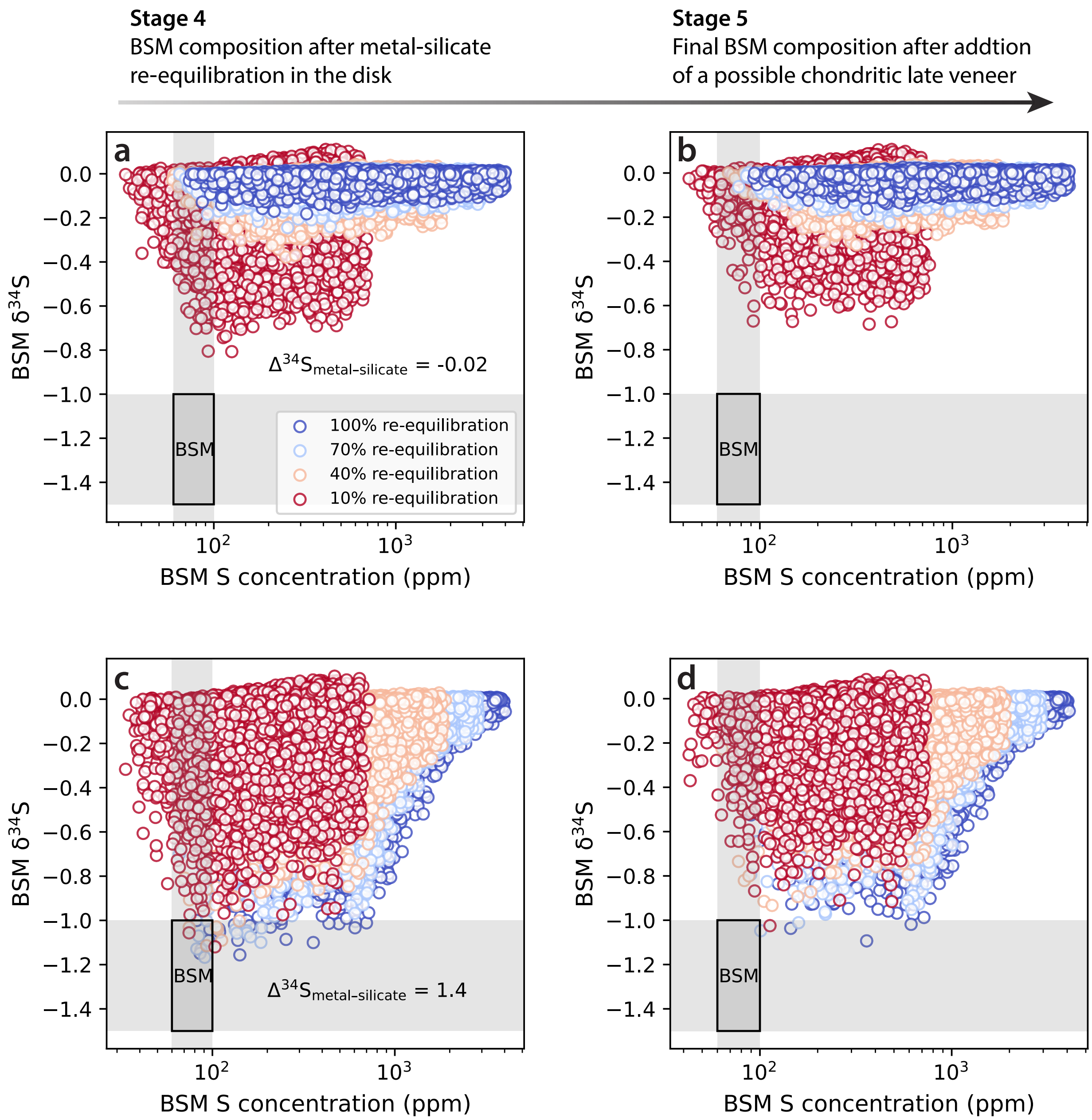

Fig. S2. BSM compositions after metal –silicate re-equilibration under varying degree of equilibration (canonical giant-impact model). The left column shows Monte Carlo simulation results for BSM compositions after metal-silicate re-equilibration, assuming $\Delta^{34}S_{metal\text{-}silicate}$ = -0.02‰[9] and 1.4‰[1,21,28] across temperatures ranging from 2,100 to 4,000 K. The right column shows the final BSM compositions after addition of a chondritic late veneer (0–0.4 wt.% of the lunar mass[31,34,36,37]). See Methods for details.

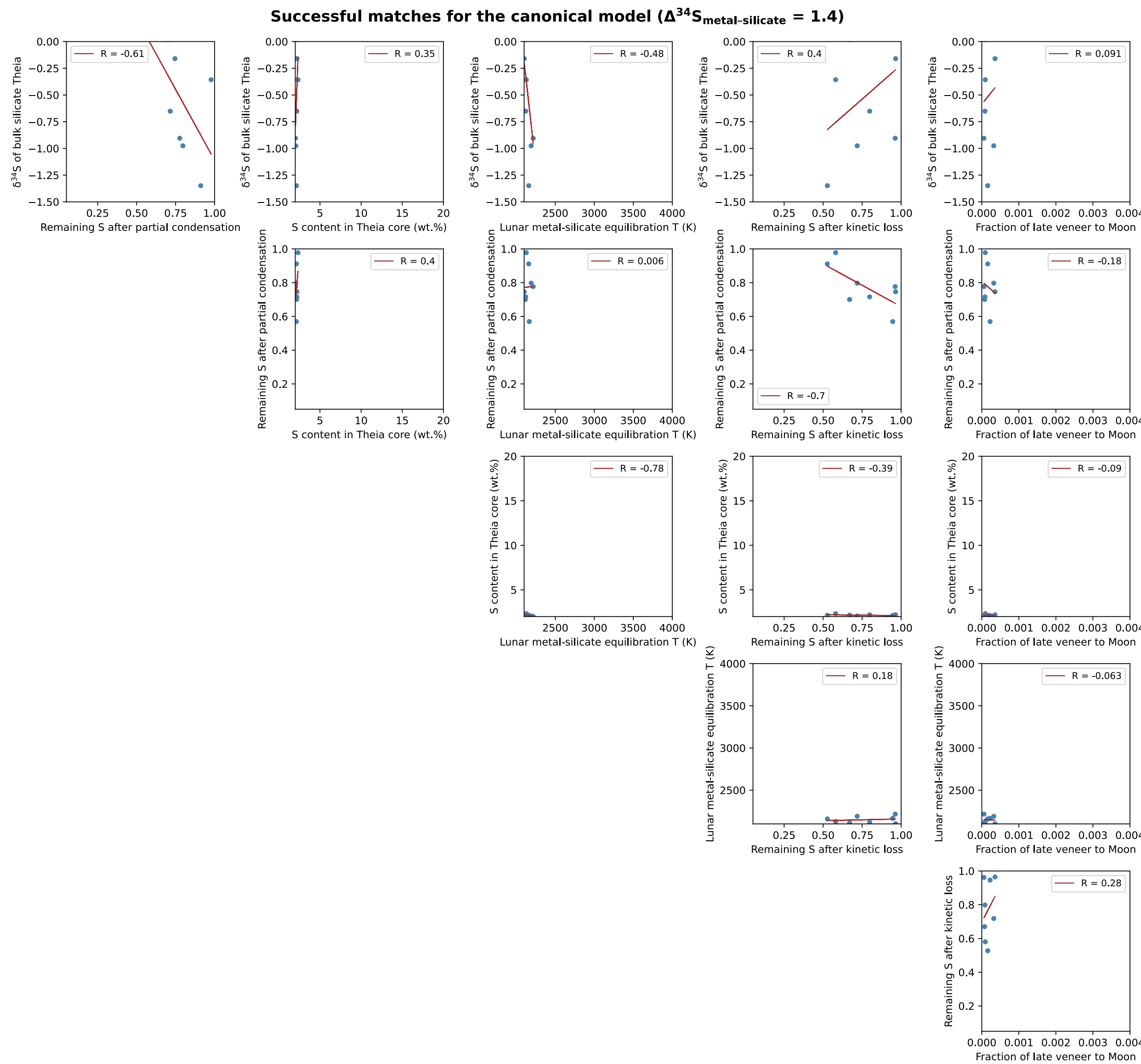

Fig. S3. Correlation plots of the parameter spaces that can simultaneously reproduce the observed S concentration and $\delta^{34}S$ composition of the BSM under the canonical giant-impact model. *R* indicates the Pearson correlation coefficient. The limited successful matches require simultaneously that: (i) $\Delta^{34}S_{metal\text{-}silicate}$ = 1.4‰[1,21,28], a large fractionation factor not yet experimentally verified; (ii) the S content in Theia's core be ~2 wt.%; (iii) the metal-silicate re-equilibration temperature be ~2,100 K; and (iv) the fraction of late veneer added to the Moon be < 0.05%. The most significant correlation is observed between the S content in Theia's core and the lunar metal-silicate equilibration temperature (*R* = -0.78); though the total allowed variations in both parameters remain narrow.

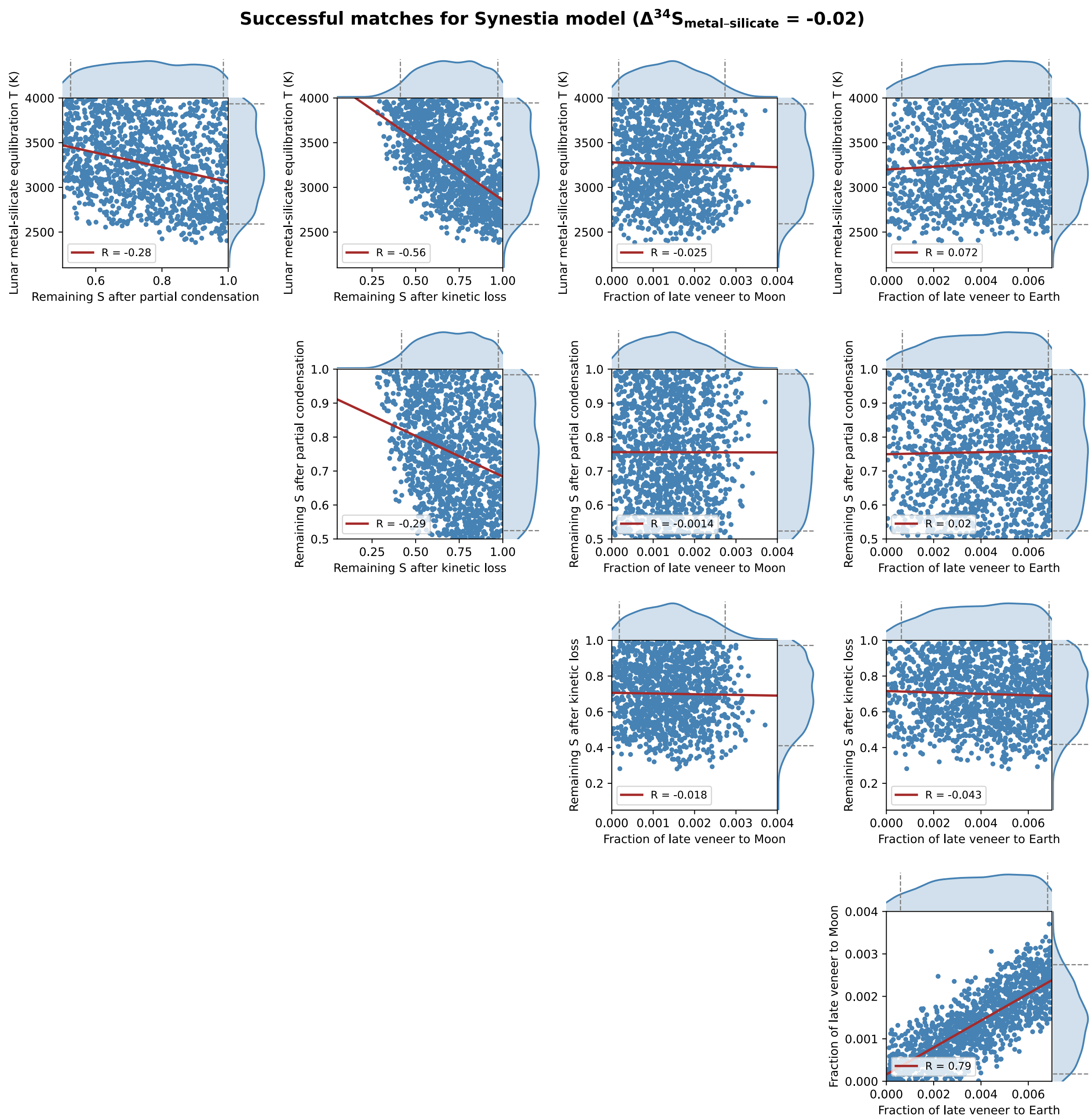

Fig. S4. Correlation plots of the parameter space that simultaneously reproduces the observed S concentration and $\delta^{34}S$ composition of the BSM under the Synestia model (assuming $\Delta^{34}S_{metal\text{-}silicate}$ = -0.02‰[9]). R indicates the Pearson correlation coefficient. The plots above and to the right of each diagram show the Kernel Density Estimation (KDE) of the probability distribution of successful matches. Dashed lines bound the central 90th percentiles, taken as representative of the matching parameter space. The lack of or weak correlations between most parameters demonstrates the broadness of matching conditions under the Synestia model in reproducing lunar BSM S and $\delta^{34}S$ compositions. A positive correlation between late-veneer additions to Moon and Earth (R = 0.79) with a slope < 1 are consistent with correlated, yet disproportional late accretion to both bodies[34–37]. A moderate negative correlation between metal–silicate equilibration temperature and remaining S after kinetic loss (R = –0.56) agrees with the expectation that higher temperatures predict greater S loss in an undersaturated vapor medium within the proto-lunar disk.

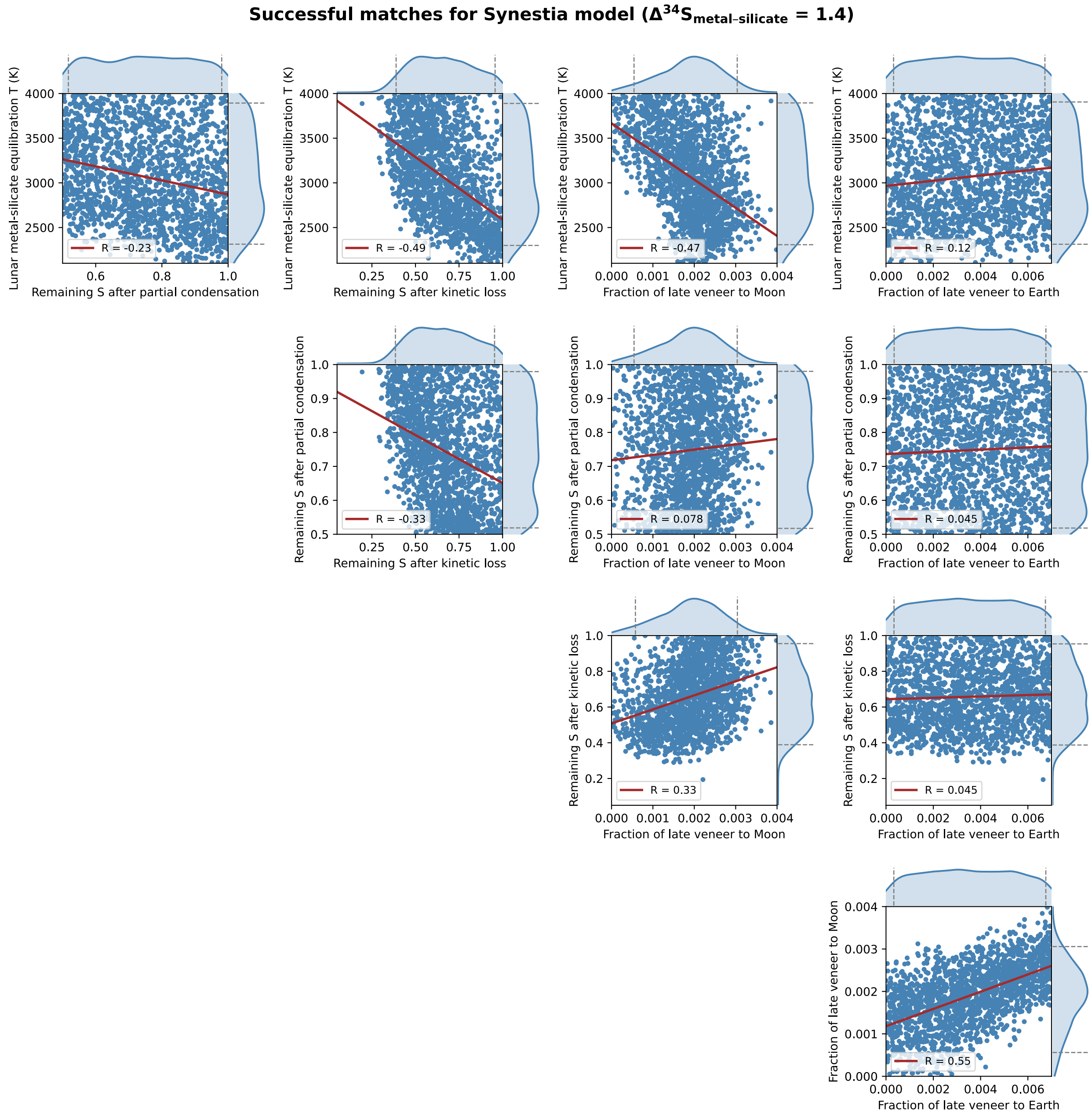

Fig. S5. Correlation plots of the parameter space that successfully reproduces the observed S concentration and $\delta^{34}S$ composition of the BSM under the Synestia model (assuming $\Delta^{34}S_{metal\text{-}silicate} = 1.4‰$[1,21,28]). *R* indicates the Pearson correlation coefficient. The plots above and to the right of each diagram show the Kernel Density Estimation (KDE) of the probability distribution of successful matches. Dashed lines bound the central 90th percentiles, taken as representative of the matching parameter space. The lack of strong correlations among most parameter pairs demonstrates the broad and flexible parameter space that allows the Synestia model to explain the BSM S and $\delta^{34}S$ systematics. A positive correlation between late-veneer additions to Moon and Earth (*R* = 0.55) with a slope < 1 support correlated, yet disproportional delivery of late-accreted materials to both bodies[34–37].

Table S1. Parameters and variables used in the Monte Carlo simulations.

Parameter	Description	Value or Range	References or Notes
For canonical giant-impact modeling			
$f_{proto-Earth}$	Mass fraction of the proto-Earth mantle in the lunar disk	0.25	Ref. [2,11,15,16]
f_{Theia}	Mass fraction of Theia mantle in the lunar disk	0.75	Ref. [2,11,15,16]
f_{core}	Mass fraction of lunar core	0.02	Ref. [10,45]
$S_{Theia-core}$	Sulfur concentration in Theia's core	20,000–200,000 ppm	Ref. [18–20]
S_{Theia}	Core-to-mantle partition factor for S in Theia	40–400 ppm	Scaled by $S_{Theia-core}$ using a factor of 500[19]
$S_{proto-Earth}$	Sulfur concentration in proto-Earth BSE	225 ± 25 ppm	Ref. [22]
$\delta^{34}S_{proto-Earth}$	Sulfur isotopic composition of proto-Earth mantle	-1.28 ± 0.33‰	Ref. [21]
$\delta^{34}S_{Theia}$	Sulfur isotopic composition of Theia's silicate	-1.5‰ to 0.5‰	
$\delta^{34}S_{Theia-core}$	Sulfur isotopic composition of Theia's core	0‰	Ref. [23,24]
χ_{eq}	Degree of lunar metal-silicate re-equilibration	0.1 to 1	
f_{pc}	Partial condensation mass retention fraction for sulfur	0.05 to 1	Ref. [3,7,8]
For Synestia modeling			
f_{LV-BSE}	Late veneer mass fraction added to the BSE	0 to 0.7%	Ref. [31,34,36,37]
$\delta^{34}S_{BSE}$	Sulfur isotopic composition of the BSE	-1.28 ± 0.33‰	Ref. [21]
S_{BSE}	Sulfur concentration in the BSE	225 ± 25 ppm	Ref. [22]
f_{pc}	Partial condensation mass retention fraction for sulfur	0.5 to 1	Ref. [3,8]
Common for both models			
N	Number of Monte Carlo simulations	300,000 for canonical model and 20,000 for Synestia model	
S_{LV}	Sulfur concentration in CI-like chondritic late veneer	20,000 ppm	Intermediate among chondrites (Ref. [44,45])
T_{eq}	Equilibrium condensation temperature	3,000 K	Ref. [7]
$\Delta^{34}S^{eq}_{vapor-melt}$	Equilibrium fractionation factor	$-113000/T_{eq}^2$	Ref. [9]
f_{pv}	Vaporization loss mass retention fraction	0.05 to 1	
$\Delta^{34}S_{metal-silicate}$	Isotope fractionation between metal and silicate	-0.02‰ or 1.4‰	Ref. [1,9,21,28]
T_{ms}	Metal-silicate equilibration temperature	2,100–4,000 K	
f_{LV-BSM}	Late veneer mass fraction added to the Moon	0 to 0.4%	Ref. [5,32–34]

Note: Random variables are sampled using uniform or normal distributions as specified in the method section.