Supplementary Material

Xuite, $Ca_3Fe_2[(Al,Fe)O_3(OH)]_3$, a new mineral of the garnet group: Implications for wide occurrence of nano-minerals

Seungyeol Lee[1,2,3,*] and Xiaofeng Guo[4,5]

[1]Department of Geoscience, University of Wisconsin–Madison, Madison, WI 53706, USA

[2]USRA Lunar and Planetary Institute, 3600 Bay Area Boulevard, Houston, TX 77058, USA

[3]ARES, NASA Johnson Space Center, 2101 NASA Parkway, Houston, TX 77058, USA

[4]Department of Chemistry, Washington State University, Pullman, WA 99164, USA

[5]Alexandra Navrotsky Institute for Experimental Thermodynamics, Washington State University, Pullman, WA 99164, USA

* Corresponding author:

Dr. Seungyeol Lee

Tel: 1-608-770-9310

Email: slee2@lpi.usra.edu

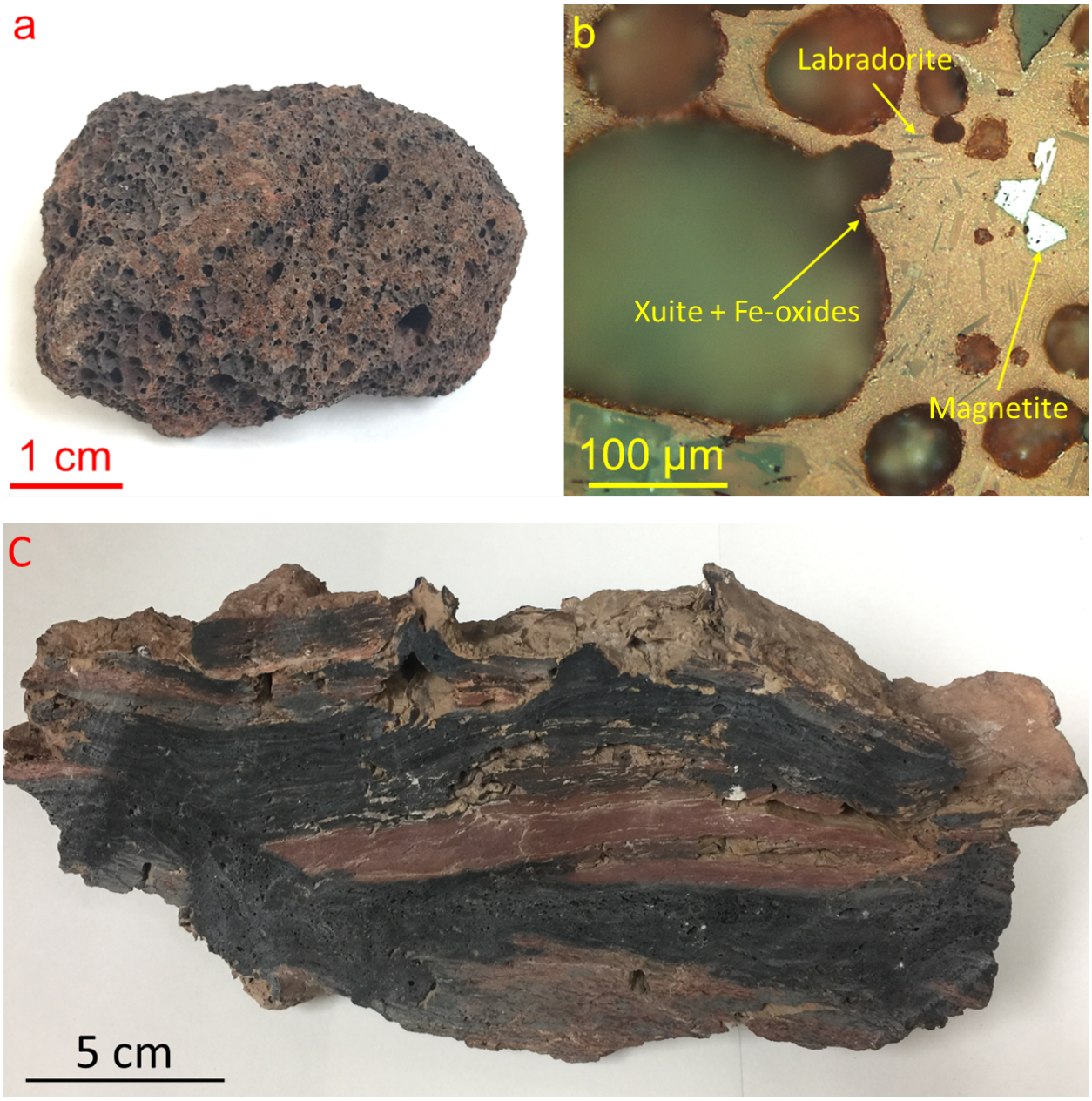

Figure S1. (A) Reddish-brown scoria hand specimen showing porous texture with vesicles covered by oxide minerals of xuite, luogufengite, valleyite, hematite and maghemite. (B) A polished surface of a scoria thin section shows brownish coating of the oxides on the vesicle surfaces. The glassy groundmass of the scoria contains crystals of magnetite and labradorite. (C) A specimen of paralava sample from Gillette, Wyoming, USA. The reddish area contains the xuite, hematite, and silica-rich glass.

Table S1. K-factors for the Phillips CM200 Ultra Twin TEM[a,b]

Element Ratio	Standard	*k*-factor ($k_{x\text{-}Si}$)
Na/Si	Albite	1.03
Mg/Si	Forsterite	0.90
Al/Si	Anorthite	0.92
K/Si	Orthoclase	0.65
Ca/Si	labradorite (Oregon)	0.66
Fe/Si	Fayalite	0.73

[a]Conditions: X-tilt = +10°, Y-tilt = 0°, Spot size = 5

[b]*k* is a sensitivity factor that relates elemental peak intensity to concentration: $C_A/C_B=k_{AB} * I_A/I_B$

Table S2. Atomic coordinates, atomic displacement parameters and site (Z_{TET}) occupancies of xuite.

Space group ($Ia\bar{3}d$): a = 12.5056(5) Å					
Atom	Occupancy	x	y	z	U_{iso}
X	$Ca_{0.92}Mg_{0.08}$	0.125	0	0.25	0.0094
Y_{OCT}	$Fe_{0.96}Ti_{0.04}$	0	0	0.5	0.0137
Z_{TET}	$Al_{0.43(4)}Fe_{0.33(3)}Si_{0.05(1)}\square_{0.19}$	0.5	0.25	0.125	0.063
φ	$O_{1.00}$	0.0351(5)	0.0594(6)	0.6459(8)	0.0219
H	$H_{0.37}$	0.1477	0.0909	0.8299	0.038

Note: The occupancy of hydrogen is calculated on the basis of charge neutrality of the refined hydrogarnet structure. The hydrogen coordinates and U_{iso} values are taken from a single-crystal X-ray diffraction study of a hydrogarnet analogue by Ferro et al. (2003).